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PREFACE

The European Conference on Modelling and Simulation is an event that is firmly established on the agenda of European simulationists but also one that attracts researchers and practitioners from much further afield. This year's conference, the 23rd ECMS, has attracted over 140 participants from 29 countries including: Austria, Belgium, Brazil, Canada, Czech Republic, France, Germany, Hungary, Iran, Italy, Jordan, Korea, Latvia, Malaysia, Malta, Mexico, The Netherlands, Norway, Poland, Portugal, Romania, Russian federation, Saudi Arabia, Slovakia, Spain, Slovenia, Tunisia, United Kingdom, United States.

The ECMS 2009 is organised around 12 thematic tracks, which highlight the breadth of relevance of computer simulation modelling methodology. It is perhaps not surprising that in the year of global recession the research theme of modelling and simulation in Finance and Economics is seen as a particularly important focus of the ECMS 2009. Other themes such as Agent-Based Simulation, Simulation of Complex Systems, Multi-Resolution and Granular Modelling, Intelligent Systems Simulation and Bond Graph Modelling provide theoretical underpinnings for the application of the methodology in a broad range of applications. In order to maximise the impact of research advances in specific application areas the contributions discussing the applications of the simulation methodology have been grouped under thematic headings of Simulation in Industry, Business and Services, Simulation Applications in Industry, Simulation in Experimental Science and Engineering, Simulation in Logistics, Transport and Supply Chains, Simulation in Electrical and Electromechanical Engineering and Simulation and Control of Technological Processes. However, the list of application areas is not exhaustive and we can see some emerging fields where the simulation modelling methodology may prove to have a very significant impact in the future. One of such areas, represented by a paper in the Multi-Resolution and Granular Modelling theme is modelling in agriculture and crop science. As we face the unknown implications of the global climate change the impact of new weather patterns on the ability to produce crops is an urgent and important challenge that simulationists should embrace.

In short, the distinguished track record of 23 years of ECMS research forum is rooted in the vibrancy of the community of simulationists in Europe and world-wide who constantly look at the global challenges that we all face. We, the organisers of the ECMS 2009 are confident that the cross-fertilisation of ideas that can be afforded through formal presentations and informal discussions will provide a step forward in tackling those challenges.

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ECMS 2009 SCIENTIFIC PROGRAM

Plenary Papers

Automatic Identification of Regression-ARIMA Models with Program TSW (TRAMO-SEATS for Windows)

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KEYWORDS Automatic modeling, very many time series, X11, regresion-ARIMA models, TSW, AMI.

ABSTRACT

Short-term economic data (say, monthly data) are subject to short-term "noise" that, if not properly discounted, can be seriously misleading when interpreting the underlying medium– or long-term evolution of the variables. Among the different types of noise, seasonal variations play a dominant role, and seasonal adjustment of economic data has indeed a long tradition. At present, every month many thousand series are routinely adjusted by data-producing agencies.

Since the appearance of the US Bureau of the Census (USBC) X11 method, adjustment of data has been overwhelmingly done with a few filters designed a priori to have some desirable property, namely, removal of the series variation associated with seasonal frequencies. However, blind application of the X11 filters presents some shortcomings. Lacking a precise definition of seasonality, one seems bound to accept as such simply the output of the filter. Yet insofar as series with no spectral peak at a seasonal frequency may well display power for that frequency (for example, a white-noise series), X11 would estimate a seasonal component for that frequency. This component would of course be spurious.

Ultimately, the seasonal component (or trend component) that a filter estimates is an estimator of an unobserved component and, as such, is contaminated by an estimation error. How large can this error be expected to be? The answer to this question is crucial for a rigorous assessment of the short-term evolution and, naturally, for proper enforcement of policies based on (explicit or implicit) targeting. For example, assume a monetary policy based on annual targeting of a monetary aggregate growth. Further, assume that in December, a growth of 8% is targeted for the next year, and in January the seasonally adjusted series shows a 10% growth (on annualized terms). Could the 2% difference be explained by the size of the measurement error? In other words, is the difference not significantly different from zero? If it is not, the interest rate instrument should be left unmoved; on the contrary, if the difference turns out to be significant, the interest rate should be increased. Clearly, it is important to avoid reacting to noise and not to the proper signal. Unfortunately, computation of the standard deviation of the seasonally adjusted series estimation error does not have a clear answer in the context of a-priori designed filters.

In the early 80's proposals were made to use Auto Regressive Integrated Moving Average (ARIMA) models, together with Signal Extraction techniques of the Wiener-Kolmogorov type to estimate signals (or unobserved components) such as the seasonally adjusted series or the trend. The ARIMA model for each series would be identified from the stochastic structure of the series, and correct specifications could be assessed with standard diagnostics. Next, a stochastic partial fractions decomposition would yield the ARIMA model for each unobserved component, and hence seasonality would be fully defined through its model. The filter, determined from the series structure, would avoid the danger of spuriousness (and, for example, no seasonality would be extracted from a white-noise series). Finally, the modelbased structure could be exploited to provide the desired inference, and in particular, the standard deviation of the signal estimation error.

This model-based method was appealing, but it confronted some serious problems. For large scale application it required very heavy doses of time series analyst resources because there were no automatic model identification (AMI) procedures that were reliable enough. Further, it seemed to require heavy computational resources because the identification and estimation algorithms available were not efficient enough. Finally, for many real series, ARIMA models had to be extended in several directions; some important ones were: the capacity to detect and remove possible outliers, possible calendar effects that are non-periodic and other possible special regression-type effects, and the capacity to handle missing observations. To be able to deal with these extensions, ARIMA models have to

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be replaced by the so-called Regression-ARIMA models. Of course, outlier and calendar effect detection, as well as interpolation, have to be incorporated to the complete AMI procedure.

In the decade of the 90's, Víctor Gómez and Agustín Maravall completed the Regression-ARIMA modelbased methodology and produced a pair of connected programs that successfully enforced the methodology. Moreover, they could efficiently and reliably treat in an automatic mode very large sets of series. In the last ten years use of the programs has become widespread throughout the world, and they are intensively used at economic agencies and institutions, research, business, and -most relevantly- in data producing agencies, where seasonal adjustment is the most widely used application. The two programs are named TRAMO ("Time series Regression with ARIMA noise, Missing values and Outliers") and SEATS ("Signal Extraction in ARIMA Time Series"); they are freely available, together with additional tools and documentation, at the Bank of Spain web site (www.bde.es).

The presentation will center on the application of program TSW to a large set of monthly time series. TSW is a Windows interface of updated versions of programs TRAMO and SEATS.

The program estimates a general Regression-ARIMA model, and computes forecasts and interpolators for possibly nonstationary series, with any sequence of missing observations, and in the presence of outliers. The program contains an option for automatic model identification, automatic detection and correction of several types of outliers, and for pretesting and estimation of Calendar-based effects. Several types of intervention or regression variables can also be included.

Next, the program estimates and forecasts the trendcycle, seasonal, calendar, transitory and noise components in the series, using signal extraction techniques applied to ARIMA models. The program contains a part on diagnosis and on inference, and an analysis of the properties of the estimators and of the estimation and forecasting errors. The last part of the output is oriented towards its use in short-term economic policy and monitoring.

TRAMO contains an extension (TERROR, or Tramo for ERRORs) to the problem of quality control of data in large data bases of time series; SEATS can be applied for estimation of long-term trends and (business) cycles. The presentation will briefly describe the methodology and, given that the model-based method relies heavily on the adequacy of the complete AMI procedure, will center on this feature. The program TSW will be applied, in its automatic mode and in real time, to a set of 500 monthly European Exports series. These series are part of a larger set of 1615 series that were provided

by Eurostat. The results for the full set will be analyzed. In particular, it will be seen that the empirical sizes of several diagnostic tests are nearly identical to the theoretical sizes.

At present, production of seasonally adjusted data by data-producing agencies is overwhelmingly dominated by TRAMO-SEATS and X12-ARIMA (the USBC successor of X11). X12ARIMA is a mixed model/filter design-based method that will eventually lead to X13-ARIMA-SEATS. (X12ARIMA has already incorporated and adapted the TRAMO AMI procedure). One is tempted to conclude that, in what concerns seasonal adjustment, a change in paradigm is taking place; the new paradigm being a model-based one.

CONTEXT-INDEPENDENT SOLVERS

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Black box optimizers have a long tradition in the field of operations research. These procedures treat the objective function evaluation as a black box and therefore do not take advantage of its specific structure. Black box optimizers have also been referred to as context-independent procedures. Figure 1 shows a schematic representation of what we mean by a black-box approach. The objective function is evaluated "outside" the solution procedure and therefore the procedure cannot exploit the structure of this objective function (and additional penalty values that the user could include to deal with infeasible solutions). What we mean by "outside" is that the solution procedure does not know anything about the objective function that it is optimizing. It only knows the values of the variables in each solution that is submitted to the black-box evaluator. Context-independent solvers do not exploit properties of the problem because they have no knowledge of specific characteristics of the objective function. For instance, it is unknown to the solver whether the objective function is linear or nonlinear and therefore it cannot apply the most effective search strategies for a given situation.

The input to the objective-function evaluator is a solution p and the output is the objectivefunction value f(p). This is the typical configuration used by heuristic methods developed for optimizing simulations, where the objective-function evaluator is replaced with a simulation model.



Figure 1: Schematic Representation of the Black-Box Approach.

When solving an optimization problem, such as the well-known traveling-salesman problem, a common practice is to develop a context-dependent method. By context-dependent, or white-box application, we mean that the procedure explicitly exploits the structure and properties of the problem in order to conduct an efficient search. Most heuristic and metaheuristic implementations are based on this paradigm, i.e., developing a specialized method for a specific problem. The main concern in this type of research is to create a method capable of competing against the best known procedure for the problem under consideration. Our current goal is different, as we attempt to create a method that finds solutions of reasonable quality for a class of problems based on a context-independent paradigm.

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) In this paper we restrict our attention to two classes of problems: (1) the class of problems whose solutions are represented by permutations (Campos et al. 2005) and (2) the class of problems whose solutions are represented by binary vectors (Gortazar et al. 2008). The first class includes a wide range of problems such as the traveling-salesman problem, the quadratic-assignment problem, various single-machine sequencing problems, and the linear-ordering problem, to mention a few. The second class includes other well known problems, such as the maximum diversity problem, the max-cut or the knapsack problems.

A black box evaluation may or may not be deterministic. Stochastic black-boxes are typically constructed as simulation models. Simulation-optimization has received a fair amount of attention in recent years. A Google Scholar search on "simulation optimization" returns more than 7,500 links to articles containing the phrase. Academic circles favor simulation-optimization approaches that are based on stochastic (gradient-based) approximations and response surface methodologies. However, modern commercial discrete-event or Monte Carlo simulation software employs metaheuristic technology as the optimization engine. The Premium Solver Platform version 7.2 of Frontline Systems, Inc (http://www.frontsys.com), for instance, includes the Standard Evolutionary solver that is a context-independent GA implementation. Opttek Systems, Inc (http://www.opttek.com) commercializes OptQuest 6.0, a context-independent solver based on scatter search. Finally a GA-based commercial implementations of general-purpose optimizers is Evolver4.1 by Palisade Corporation (http://www.palisade.com).

The main contribution of our work is the development or adaptation of scatter search methods that are helpful in the solution of permutation and binary problems for which the objective function is treated as a black-box evaluator. The performance of our procedure has been assessed using different set of instances of different permutation and binary problems. The solutions obtained with the proposed procedure have been compared with both the commercial programs mentioned above and with the best known solutions to each problem.

Vicente Campos, Manuel Laguna and Rafael Martí (2005) Context-Independent Scatter and Tabu Search for Permutation Problems, *INFORMS Journal on Computing*, 17(1) 111-122.

Francisco Gortazar, Abraham Duarte, Manuel Laguna and Rafael Martí (2008) Context-Independent Scatter Search for Binary Problems, *Technical Report* 08, University of Valencia.

Simulation in Industry, Business and Services

BUSINESS MODEL DESIGN USING BUSINESS PROCESS MODELLING: Case of Slovenian Transport Logistics Cluster creation

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KEYWORDS

SCM, e-logistics, cluster, business model, business renovation.

ABSTRACT

the pursuit of enhanced competitiveness In organisations are today searching for innovative business models in order to foster economic benefits. In Slovenia, several clusters are being formed, including the Slovenian Transport Logistics Cluster (STLC) as one of the most important. The STLC is currently in the stage of dynamic growth, demanding business model formation and adequate informatisation. The main goal of the paper is to present the STLC business model creation, bridging the gap between Supply Chain Management (SCM) and e-Logistics. The business model creation is presented in several phases. The first phase involves business modelling of the existing business processes of organisations (AS-IS model). The results of the first phase allow an in-depth view of the STLC that is used in the future in the business model setup. Next, TO-BE processes are created which are to be implemented and supported via informatisation. Business model should enable homogenous and transparent business activity between cluster members. The purposes of the business model creation is to standardize business processes, allow cost cutting and improve business performance, reduce operating times, support asset management, and trace shipments which are the basics of economic competitiveness.

INTRODUCTION

Tougher competition in all industrial sectors sharpened by globalization and the fall in global supply is forcing companies to optimize their business processes and adopt new ways of achieving mergers or partnerships that directly lead to lower business costs. With these strategic alliances new management strategies are being formed, such as clusters, Supply Chain Management (SCM), e-logistics etc. Some authors suggest that logistics are 'worth' 10% to 12% of Gross Domestic Product-GDP (Sahay, 2003). According to AMR research (Challener, 2001), e-logistics has the

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) potential to cut costs by 10%. Based on these two references we can conclude that e-logistics can save our money by up to 1.2% of GDP. It is therefore no surprise that in the last few years' top management in highly effective companies such as Hewlett-Packard, Compaq, Digital Equipment Corporation, Xerox, Dell and Benetton Group has been in favor of the supply chain and therefore e-logistics (Romano, 2003).

There is a collection of literature indicating the importance of clusters and networks not only between firms, but along the value chain and across industries. The networks involved in these clusters are integral to knowledge generation and diffusion, technology transfer, sharing risks and costs, allowing firms to access new markets and opportunities and, finally, building a comparative advantage in the global market. Porter (Porter, 1990) defines clusters as geographic concentrations of interconnected companies, specialized suppliers, service providers, firms in related industries, and associated institutions. He proposes a model that provides conditions that have to be met for a firm to be internationally competitive and successful. This model focuses on four primary conditions which he arranges in a diamond-shaped diagram: factor conditions, demand conditions, structures of firms and rivalry and related and supporting industries. The 'Related and Supporting Industries' feature of the diamond denotes the importance of clustering for developing an international competitive advantage incorporating two features of a healthy cluster: the presence of vertical support through internationally competitive supplier industries which ensure costeffective and speedy deliveries; and the presence of horizontal support in internationally competitive related industries to co-ordinate and share activities with and to stimulate local competition.

In this article STLC business model setup will be presented through the project called "The Modeling, Analyzing and Renovation, Standardization and Informatisation of Business Processes of the Slovenian Transport Logistics Cluster", which is being carried out by the Business Informatics Institute of the Faculty of Economics at the University of Ljubljana, Slovenia. Informatisation offers logistics companies not only better connectivity with their customers and suppliers but also improved performance and faster responses.

For all logistics companies it is assumed that they control the global logistics chain of their customers and therefore depend on the successful implementation of information technologies which leads to lower inventory costs, better customer retention, asset management etc.

THE TRANSPORT LOGISTICS CLUSTER IN SLOVENIA

The STLC was formed to compete with the European logistics market. It is an association of 12 companies and 3 institutions: freight forwarding and shipping agencies, port services, ecological and university research institutions. Currently, transportation-logistics service suppliers within the STLC prepare common programmes, market presentations, education equipment acquisitions and complete service developments. The STLC's vision is to create comprehensive conditions for its members that enable them to offer full logistical support above and beyond the Slovenian transportation route relative to the markets of Central and South-east Europe. Slovenia is encountering fiercer competition by virtue of it having joined the European Union on 1 May 2004 and it is only through harmonious co-operation between the companies associated in the STLC that they can succeed in the European market.

Slovenia has all the attributes of a distribution and logistics hub: a fortuitous geographical position at the heart of the region intersected by traditional trade and transport routes – the location of choice for international companies planning their future regional distribution set-up.

Two pan-European transport corridors (No. 5 linking Barcelona and Kiev, and No. 10 from Salzburg to Thessalonica) intersect in Ljubljana, the capital of Slovenia. Slovenian companies' excellent track record in the logistics business coupled with modern transport infrastructure is a proven recipe for high-quality and cost-competitive services tailored to clients' needs. As an EU member state Slovenia is a gateway for Asian and EU manufacturers and traders to faster and more reliable trade routes that meet at fully equipped logistics centers.

Shipping to Slovenia's only cargo port – the Port of Koper – means gaining 7 to 10 days for ships arriving from Asia compared to sailing to Europe's northern ports. Its total maritime throughput is about 15 million tones. There are currently 11 modern, fully equipped terminals specializing in various types of goods, storage faculties for general cargo and several special warehouses. Special advantages are available in the 4.7 sq. km. of the port's economic zone with its 324,000 sq. m. of covered and sheltered warehouse facilities and slightly less than 1 million sq. m. of open-air storage.

The motorway density in Slovenia is higher than the EU-25 average and the links with the neighboring EU member states and South-east Europe are equally good. Currently, there are over 500 km of well-maintained motorways and 1,050 km of trunk roads. The extended motorway network is scheduled for completion by 2013.

As the railway service is regaining its importance, modernization of this infrastructure is one of the national priorities. Freight traffic is well-developed while the rail links between the Adriatic Sea and the landlocked CEE countries offer many opportunities. Both freight and passenger services with South-east Europe have expanded in the last few years. The national rail operator Slovenian Railways (SŽ) runs both passenger and freight services and possess a railway infrastructure, including 60,000 sq. m. of warehouse space.

Three international airports provide easy access by air to Slovenia. The central Slovenian airport and cargo facility is Aerodrome Ljubljana located 25 km from the capital. Scheduled flights operated by several airlines carry passengers to important European destinations. The airport was recently renovated, its infrastructure extended and the cargo terminal modernized. Maribor Airport mostly handles cargo transport whereas Portorož Airport only has facilities for smaller planes.

Slovenia is well situated to serve the markets of Central, Eastern and South-east Europe. Thanks to its strategic geopolitical position and decades of close economic ties with its neighbors, Slovenian companies are true connoisseurs of the regional markets. This also includes knowledge of the various languages, differences in legislation and, particularly, mentality along with a business culture in specific areas which originates from personal ties maintained over many years.

Transit traffic has always played an important role as traditional transport. As traditional trade routes are being reopened, there is a clear upswing in road and rail transport services. Further, Slovenian transport and logistics companies have been proactive in the last few years in exploiting investment opportunities in Southeast European markets where Slovenia is one of the most important foreign investors.

Slovenian freight forwarders, carriers and warehouse operators have up-to-date fleets of vehicles and mechanized and computerized warehouses with stateof-the-art technology. Ever more firm offers their customers modern logistics hubs, along with the possibility of outsourcing complete logistics services. The number of companies specializing in transport services forging strategic links is rising and the focus on transport is broadening to include the full range of logistics activities. Slovenian logistics companies and related organizations are joining forces in the TLC.
New warehouse facilities and distribution centers are being built to satisfy requirements following Slovenia's accession to the EU as warehouses in areas bordering other EU countries are being used in the transit business

(http://www.investslovenia.org/industries/logistics and distribution/, 2008).

The reason underlying the STLC's creation is the growth in TLC formations worldwide, especially in Europe (Figure 1). From the STLC's point of view the following European TLCs are especially relevant since they represent direct competition:

Seine-Normandie Logistics Cluster

(http://investmentinnovation.wordpress.com/2007/11/1 4/seine-normandie-logistics-cluster-best-practice/)

Cluster Transport Logistique Wallonie Belgium (http://clusters.wallonie.be/transport-logistique/en/) Unitrans Holdings

(http://www.unitrans.co.za/content/operation freight 1 ogistics.asp)

Turku Logistics Cluster



Figure 1. European TLCs

SUPPLY CHAIN MANAGEMENT, LOGISTICS AND E-LOGISTICS

With the development of information technologies and information knowledge it was discovered that SCM and e-logistics have a close connection with logistics. The successful integration of SCM depends on the implementation of e-business in logistics, called elogistics. Later these two terms are reflected in the system of e-logistics which, along with the use of modern information technology, complements SCM and logistics.

SCM as a management category has strongly evolved in the last few decades, introducing several key issues spanning from the strategic to the operational level (Simchi-Levi et al., 2005):

the strategic level deals with decisions with a longlasting effect on the firm. This includes decisions regarding the number, location and capacity of warehouses and manufacturing plants, as well as the flow of material through the logistics network.

the tactical level includes decisions typically updated anywhere between once a quarter and once a year. These entail purchasing and production decisions, inventory policies and transportation strategies including the frequency with which customers are visited.

the operational level refers to day-to-day decisions such as scheduling, lead-time quotations, routing, and truck loading.

In this paper we introduce and discuss business process modeling and renovation as a methodology that supports TLC members in their strategic-level decisions.

Supply Chain Management

In the last few years companies have been increasingly realizing that the efficiency of their business depends heavily on collaboration and co-ordination with their suppliers and customers (Hieber, 2002). In order to boost their competitiveness they carefully manage the supply chain.

A supply chain is the stream of processes involved in moving goods and services from the customer order through the raw materials stage, supply, production, and distribution of products to the customer. All organizations have supply chains of varying degrees depending on the size of the organization and type of product manufactured. These networks obtain supplies and components, change these materials into finished products and then distribute them to the customer.

Managing the chain of events in this process is what is known as Supply Chain Management. Effective management must involve coordinating all the different links in this chain as quickly as possible without losing any quality or customer satisfaction, while still keeping costs down.

According to Chopra and Meindl (Chopra and Meindl, 2001), a supply chain consists of all the stages involved, directly or indirectly, in fulfilling a customer request. A supply chain not only includes the manufacturer and suppliers but also transporters, warehouses, retailers, and customers themselves. Within each organization, such as a manufacturer, the supply chain includes all functions involved in meeting a customer's request. These functions include, but are not limited to, new product development, marketing, operations, distribution, finance, and customer service. Further, Supply Chain Management entails the design, maintenance and operation of supply chain processes to the satisfaction of end users.

Within a TLC a supply chain is organized through transporters, transport organizers, warehouses and financial operators. An orderer no longer looks for the cheapest transportation but the cheapest transport option seeks the chance to execute an order. Integration of the SCM philosophy in logistics processes naturally calls for an advanced information system that connects all companies involved in a TLC and provides them with the appropriate information needed for bidding and, from the customers' aspect, allows the electronic ordering of logistics services.

Logistics

The main suggestion concerning the origin of logistics as a scientific discipline in economics stems from Oscar Morgenstern. The essence of Morgenstern's theory is:

'Logistics activity offers exactly defined quantities of assets and serves for each branch which needed these assets and serves in order with their intention to sustain branches at the same level in present or in higher position in the future. This leads from the origin and must be orientated or with other words transformed in space and time to reach the whole realization of these branches.'

As a science, up until the Second World War logistics only served military purposes. After the Second World War logistics became a civil science. Since then we can find many different definitions, including that given by Cooper (Cooper, 1993): the intention of logistics is to (in terms of order, quantity, quality, space and time) carry out the transportation of goods relative to the need to supplement business processes. It is intended for planning processes, executing and controlling the flow of goods, warehousing and managing information from the production of goods through to selling them to the final customer with the aim to satisfy the customer.

Logistical costs have an important influence on the pricing of a product. This was shown in a survey in which 200 European companies participated. The results were that logistics costs make up between 7.7% and 22% of the final price of products (Kettinger et al., 1997). The research shows there is much cost-saving potential in logistics processes and a possible step is to consider logistics as part of the supply chain. Hence we can confidently rely on the following definition: logistics is that part of the supply chain process that plans, implements and controls the efficient, effective flow and storage of goods, services and related information from the point of origin to the point of consumption in order to meet customers' requirements (Auramo et al., 2002).

E-logistics

It is difficult to define e-logistics comprehensively because the potential impact of e-business on logistics and Supply Chain Management is still not fully understood. One possible definition is that e-logistics simply means the processes needed to transfer goods sold over the Internet to customers (Auramo et al., 2002). Another and more sophisticated view is that elogistics is a wide-ranging topic related to supply chain integration that has the effect of eliminating intermediaries (such as wholesaler or retailers) and fosters the emergence of new players like logisticians whose role is to adapt traditional logistics chains to take the requirements of e-business into account.

If we consider it more broadly, e-logistics means doing e-business within a TLC between companies (B2B) and outside of it between the TLC and customers (B2C) over the Internet. This whole integration of e-business ensures that from the outside, a TLC looks like one company even though it is composed of many. If we want to implement the e-logistics philosophy in all companies inside a TLC we must renovate their business processes. Renovated processes are the basis for implementing e-logistics through logistical processes and are necessary for results that will reflect an improvement through the added value chain. Figure 2 shows how a supply chain and logistics with appropriate information satisfy customers. To ensure an appropriate information flow from customers to suppliers, among suppliers and among customers, a TLC needs comprehensive e-logistics.



Figure 2. Structure of a TLC

THE ROLE OF INFORMATION TECHNOLOGY IN SCM

Information technology (IT) is an important enabler of effective SCM. Much of the current interest in SCM from the IT point of view is motivated by technological

solutions that enable an SC change and the abundance of data an SC has to manage in order to manage operations effectively. IT is most commonly viewed as a support function in SCM since it spans all building blocks of the SC. IT provides a competitive advantage for many SCs. When applying SC strategies that reduce cost and lead times and improve service levels, the timeliness and availability of relevant information is critical. In addition, a growing number of companies are providing value-added IT-based services to their customers as a way of differentiating themselves in the and strong marketplace, developing long-term relationships with their customers.

The role of IT is not limited to its support function. In this article, business process modeling has been used in order to articulate and simulate possible business model proposals for the STLC.

The main purpose of developing and analyzing business process models is to find revenue and value generators within a value chain or a business model's value network. There have been a number of attempts to formally describe and classify a business process model. Venkatraman et al. (Venkatraman et al., 1998) defined a business process model as a coordinated plan to design strategy along three dimensions: customer interaction, asset configuration and knowledge leverage (Venkatraman, 2000).

A business process model is an abstraction of a business that shows how the business components are related to each other and how they operate. Its ultimate purpose is to provide a clear picture of the enterprise's current state and to determine its vision for the future. There are several reasons for producing business process models:

• A business process model helps us understand the business: a primary goal of business process modeling is to expand our understanding of the business and to facilitate communication about the business.

• A business process model is a basis for creating suitable information systems: descriptions of the business are very useful for identifying the information systems needed to support the business. Business process models also act as a basis for engineering requirements when a particular information system is being designed.

• A business process model is a basis for improving the current business structure and operation: since it shows a clear picture of the business current state a business process model can be used to identify the changes required to improve the business.

• A business process model provides a polygon for experiments: a business process model can be used to experiment with new business concepts and to study the implications of changes for the business structure or operation.

A business process model provides a basis for identifying outsourcing opportunities; by using a business process model the core parts of a business system can be identified. Other parts considered less important can be delegated to external suppliers (Trkma et al., 2007).

BUSINESS MODEL OF STLC

A business model may be defined as a model of a company while doing business in a certain environment while a certain environment is everything that influences the business processes of a company, such as buyers, suppliers etc. It also shows a system that firstly enables the implementation of business processes in terms of providing added values or goods to clients or users, secondly provides different users at different levels inside the company with the optimal quantity of information and instructions needed to carry out individual procedures or work processes and activities and, thirdly, gives stakeholders an assurance of capital stability and capital profitability.

A business model determines the business rules which everybody must be able to abide by. In our case, these rules must be followed by the STLC members, which are: Viator & Vektor d.d., Intereuropa d.d., BTC d.d., Slovenske Železnice d.d., Luka Koper d.d. and Fersped d.d. To build the STLC business model we must determine an AS-IS model which shows the present business processes of all STLC members. Many different methods and techniques can be used for modeling business processes in order to yield an understanding of possible scenarios for improvement (Ould, 1995). IDEF0, IDEF3, Petri Nets, System Dynamics, Knowledge-based Techniques, Activity Based Costing and Discrete-Event Simulation are only some examples of widely used business process modeling techniques (Eatock et al., 2000). As noted by Homes (Hommes and Reijswoud, 2000) the rising popularity of business process modeling results in a rapidly growing number of modeling techniques and tools. However, most simulation software implements a model using the discrete-event method. In Kettinger et al. (Kettinger et al., 1997) an empirical review is given of existing methodologies, tools and techniques for a business process change. The authors also develop a reference framework to assist in the positioning of tools and techniques that help in re-engineering the strategy, people, management, structure, and technology dimensions of business processes. However, relevance is far more important than completeness (Davenport and Prusak, 1998) and simple models are far more understandable by non-specialists. Process modeling tools must be capable of showing interconnections between the activities and allowing a decomposition of the processes. These tools must help users conduct 'what-if' analyses and identify and map no-value steps, costs, and process performance (bottleneck analysis). They should be able to develop AS-IS and TO-BE models of business processes which represent both existing and alternative processes. They must be validated and tested before their implementation. They can be used to predict characteristics that cannot be directly measured, and can also predict economic and performance data that would otherwise be too expensive or impossible to acquire.

For the purpose of the project we used the Flowchart technique with the Optima! tool. Figure 3 shows the components of the business process.



Figure 3. Symbols used in the Optima! tool

If we look at the AS-IS model (Figure 4) of Viator&Vektor d.d. as one of the members of the STLC we can notice five general processes: Order Acceptance, Organization of transportation, Realization of transportation, Forwarding and Warehousing. The organization of transport further (Figure 5) consists of Organization of transport with own transportation, Organization of transport with transportation of STLC members and Organization of transport with cutsourced transportation. Other members of the STLC have a similar structure of their general business processes.



Figure 4. General processes at Viator&Vektor d.d.



Figure 5. The subprocess of the Organisation of transportation

The organization of transport at Viator&Vektor d.d. (Figure 5) involves three different processes for the same task. The processes presented in Figures 4 and 5 for Viator & Vektor are also executed in the other organizations in the STLC. The main problem is that these processes are executed in each organization in a different way. The main goal of the project is thus straightforward – the standardization and renovation of the existing processes.

The organizations involved in the STLC differ in the effectiveness of their different processes from order acceptance through to the realization of transport. In the STLC we must consider if the specialization of organizations is better than their generalization. Which ever decision the STLC will take, it should be properly backed up with an analysis of the business model and organizational changes, execution times, and business process changes.

CONCLUSION AND FUTURE WORK

The goal of our project is creation of a business model, process renovation along with the examination and reengineering of current business policies procedures and activities. We believe the new paradigm can only be supported by:

• creating an environment of technology, enlightenment and receptivity;

• treating this as a holistic organizational transformation, not a technical issue;

• challenging the core assumptions and value propositions; and

• proactively establishing a distinctive Internet presence.

This case has confirmed that the analysis and carefully applied simulation of business processes is useful since it provides an insight into policies, practices, procedures, organization, process flows and, consequently, shifts people's minds from functional to process organization.

The project of "The Modeling, Analyzing and Renovation, Standardization and Informatisation of business processes of the Slovenian Transport Logistics Cluster" is in the first phase of generating an AS-IS model. Future work will focus on renovating the AS-IS model and create an appropriate TO-BE model on which a business model can be built.

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Some Models Parameters Calculation for Simulation of Network Traffic Marginal Distribution and Self-similarity

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ABSTRACT

In this paper, we present a simple numerical method of parameters calculation for well known traffic models $M/G/\infty$ Input and On-Off Sources, which allows to simulate both self-similar properties and marginal distribution of real network traffic. Some modifications of these models are considered. These modifications allow to simulate network traffic with several important statistical characterizes, such as marginal distribution, autocorrelation function and Hurst parameter like in real network traffic.

Categories and Subject Descriptors

I.6.5. [**Computing Methodologies**]: Simulation and Modeling – *Model Development*

General Terms Algorithms, Experimentation

Keywords

Self-similar Traffic, Traffic Simulation, $M/G/\infty$ Input, On-Off Sources, Long Range Dependence, Heavy-tailed Distribution

1. INTRODUCTION

We present simple algorithms of parameters calculation for two structural models, which allows to simulate both selfsimilar properties and marginal distribution of real network traffic. By structural models we assume models which is not only mathematical constructs to yield necessary characteristics, but construction which reflects nature of network traffic. Parameters of such models usually have clear practical sense, suitable for purposes of simulation, prediction, performance evaluation and so on.

Modern network traffic has two important features: first is that the traffic is result of simultaneous information exchange between large number of sources and destinations, and second is that this information exchange can have very different parameters for different pairs source-destination.

We consider two of well known modern traffic models, which directly reflects these features: $M/G/\infty$ Input and On-Off Sources. In both of them network traffic is the sum of

information flows from many sources, and total traffic characteristics depend upon of features of individual sources parameters. For example, such interesting feature of modern network traffic as self-similarity is the consequence of a fact, that duration of information exchange between one source and its destination can be considered as random value with heavy tailed distribution.

Goal of this report is to present simple numerical algorithms for calculation of individual source characteristics, which provides given marginal distribution and self-similarity of total traffic. Examples of marginal distribution and Hurst parameter of real traffic we get from some traces of Internet Traffic Archive [1].

Self-similarity of modern network traffic attracts a lot of researches attention during last two decades (see, for example, comprehensive review and collection of important results [2]). There are many successful and well known approaches to self-similar traffic modeling, like multi-scale models and fractal noise models (see, for example, resent works [3-4]). But among them $M/G/\infty$ Input and On-Off Sources models remain important and attractive for practice.

One of the first articles about models considered in this report is [5]. It is impossible to mention all the important works in this field, so just for examples of article about self-similar traffic modeling by $M/G/\infty$ Input and ON-OFF sources models let us mention a few: [6-10].

2. EXPERIMENTAL MATERIAL PREPARATION

For our experiments we took four well known traces: BC-pAug89.TL, BC-pOct89.TL, LBL-PKT-5.TCP, dec-pkt-2.tcp. First two of them are Ethernet traces from Bell Laboratories [11], others – TCP traces from Lawrence Berkeley Laboratory and Digital Equipment Corporation [12].

All these traces are a sets of records about information packets transfers through some point of appropriate networks. We consider discrete time models, therefore we need to transform these traces into realizations of discrete time random processes. We take time slot duration of 10 ms, and a value of the process at some discrete time moment is a sum of sizes of all packets arrived during

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) appropriate time slot. For practical purposes and for simplification of calculations we also scale these processes by division its values on some constant and round up the results. In practice of modern networks we don't need a one byte accuracy, so for this work our scale coefficient was 64. So, random processes under consideration are discrete time integer valued processes.

Marginal distributions of these processes are estimated by histogram method, and Hurst parameters are estimated by aggregate variance method. So, below we will assume, that Hurst parameter H and marginal distribution $Pr{Y_t=k}$ for k=0,1,... of traffic process Y_t are given.

3. $M/G/\infty$ INPUT MODEL

In this model, a random value of new sources arrives into system each time slot. Numbers of new sources in all time slots are i.i.d. random values with generic random value ξ , which has Poisson distribution with parameter λ .

In opposite to the simplest case, when all sources have the same information rate, we consider the case, when the rate of different sources can be different. It gives opportunity to get necessary marginal distribution of total traffic. So, rates of each new source at the moment of its arrival are realizations of i.i.d. random values with generic integer random value ζ , with some distribution, which we are going to find below. Each source keeps this information rate during all its lifetime in the system. After end of its lifetime the source leaves the system forever.

Lifetimes of all sources are realization of i.i.d. random values with generic integer random value τ , which has heavy tailed distribution

$$\Pr\{\tau = k\} = \frac{A}{k^{\alpha}}, \quad 2 < \alpha < 3, \quad k = 1, 2, \dots \quad (1)$$

As shown by many authors (see, for example, [2] and [8]), such lifetime distribution provides self-similarity (second order asymptotical self-similarity) of total traffic (which is the sum of the flows from all active sources) with Hurst parameter H= $2-\alpha/2$. So from given H we get α as

$$\alpha = 4 - 2H \,. \tag{2}$$

3.1 Some previous analytical results

As shown in [13], it is easy to get equation for probability generation functions (p.g.f.) of traffic distribution $\Phi_{Y}(z)$ and source rate distribution $\Phi_{\zeta}(z)$. If

$$\Phi_{Y}(z) = \sum_{k=0}^{\infty} \Pr\{Y_{t} = k\} z^{k}, \ \Phi_{\zeta}(z) = \sum_{k=0}^{\infty} \Pr\{\zeta = k\} z^{k}$$

then taking under consideration that for stationary traffic process in each time slot the number of active sources N_t is Poisson random value with parameter $\Lambda = \lambda * E \tau$, it is easy to get

$$\Phi_{\gamma}(z) = \sum_{k=0}^{\infty} \Pr\{N_t = k\} (\Phi_{\zeta}(z))^k = e^{\Lambda(\Phi_{\zeta}(z)-1)},$$

and

$$\Phi_{\zeta}(z) = 1 + \frac{1}{\Lambda} \ln \Phi_{\gamma}(z)$$

If *no fictive sources* condition is assumed, which means that

$$\Pr\{\zeta = 0\} = 0 \tag{3}$$

and leads to $\Phi_{\zeta}(z) = 0$, then in some particular cases this equation can be solved analytically and has unique solution. For example, if Y_t is assumed to have Pascal distribution with parameters m and θ , then

$$\Phi_{\zeta}(z) = 1 + \frac{1}{\Lambda} \ln \frac{(1-\theta)^m}{(1-\theta z)^m} = 1 + \frac{m}{\Lambda} \ln \frac{1-\theta}{1-\theta z},$$

and *no fictive sources* condition gives $\Lambda = -m \ln(1-\theta)$ and

$$\Pr{\{\zeta = k\}} = -\frac{1}{\ln(1-\theta)} \frac{\theta^{k}}{k}, \quad k = 1, 2, \dots$$

Unfortunately, marginal distribution of real network traffic is not even close to Pascal or any other analytically defined distribution, so below algorithm from [13] for numerical solution is presented.

3.2 Numerical calculation of source rate distribution Let us denote

$$p_k = e^{-\Lambda} \frac{\Lambda^k}{k!} \,. \tag{4}$$

Then no fictive sources condition gives

$$\Pr\{Y_t = 0\} = \Pr\{N_t = 0\} = p_0 \tag{5}$$

from which

$$\Lambda = -\ln(\Pr\{Y_t = 0\}) \tag{6}$$

By definition and according to *no fictive sources* condition, random value ζ can take only integer values starting from 1. Taking this fact into consideration, we can write down that

$$\Pr\{Y_t = 1\} = p_1 \Pr\{\zeta = 1\}$$

and



Figure 1. Traffic Distribution for LBL-PKT-5.TCP trace

$$\Pr\{\zeta = 1\} = \frac{\Pr\{Y_t = 1\}}{p_1}$$

On the same way we have

$$\Pr\{Y_t = 2\} = p_1 \Pr\{\zeta = 2\} + p_2 \Pr\{\zeta_1 + \zeta_2 = 2\}$$

where ζ_1 and ζ_2 are i.i.d. random values with the same distribution as ζ . It means that minimal value both of ζ_1 and ζ_2 is 1, so

$$\Pr{\{\zeta_1 + \zeta_2 = 2\}} = \Pr{\{\zeta_1 = 1, \zeta_2 = 1\}} = (\Pr{\{\zeta = 1\}})^2$$

and

$$\Pr{\{\zeta = 2\}} = \frac{\Pr{\{Y_t = 2\}} - p_2(\Pr{\{\zeta = 1\}})^2}{p_1}$$

Similar considerations give expression for general case:

$$\Pr\{\zeta = k\} = \frac{\Pr\{Y_t = k\} - \sum_{m=2}^{k} p_m \Pr\{\sum_{n=1}^{m} \zeta_n = k\}}{p_1}, (7)$$

where $\Pr\{\sum_{n=1}^{m} \zeta_n = k\}$ can be found as appropriate term

in m-times discrete convolution of sequence $Pr{\zeta=1}$, $Pr{\zeta=2}$, ..., $Pr{\zeta=k-m}$, which is initial part of source rate distribution found on previous iterations (7).

Equations (5)-(7) are iterative procedure to find source rate distribution numerically. Last parameter, which is necessary to find for the model is

$$\lambda = \frac{\Lambda}{E\tau},\tag{8}$$

where $E\tau$ is calculated also numerically from (1) and (2).



Figure 2. Traffic Distribution for DEC-PKT-2.TCP trace

There are two problems in practical calculation according (7): possible negative results of some iterations and when to stop these iterations. As solution for first problem, we used obvious approach: if some iteration according (7) gives negative value, appropriate probability (which is used for next iterations) is made equal to 0. Iterations are stopped, when sum of probabilities becomes close to 1 less then on 10^{-6} , and last probability is made equal to difference between 1 and sum of previous probabilities.

3.3 Numerical results for M/G/∞ Input model

Using H and $\Pr{Y_t=k}$ from real traffic traces in equations (1)-(8) we found α , λ and sequence of source rate probabilities $\Pr{\zeta=k}$. All these parameters were substituted into program of traffic simulation by $M/G/\infty$ Input model. For simulated traces of length 360000 time slots, Hurst parameters and marginal distribution were estimated by the same methods as for real ones. For TCP traces comparison of these results with real ones are shown on Figures 1 and 2, and in Tables 1 and 2. Source rates for both traces are shown on Figures 3 and 4. It looks like $M/G/\infty$ Input model works well for these kind of traces.



Figure 3. Source Rate Distribution for LBL-PKT-5.TCP trace

But for Ethernet traces the situation is much worse (see Figures 5 and 7 in next section). It could be several possible explanations of these facts. One of them is follow: modeling of new sources arrival as Poisson process is not suitable enough for local networks. In next section we consider another well known model, which is close to $M/G/\infty$ Input model, but with different assumptions about number of sources in the system.



Figure 4. Source Rate Distribution for DEC-PKT-2.TCP trace

Table 1. LBL-PKT-5.TCP trace parameters comparison

Trace	Н	Average	Variance
Real	0,666	2,017	30,545
Simulation	0,748	2,076	31,112

 Table 2. DEC-PKT-2.TCP trace parameters

 comparison

Trace	Н	Average	Variance
Real	0,755	49,528	2384,076
Simulation	0,771	46,592	2095,209

3.4 Approximation of normalized autocorrelation function

In addition to Hurst parameter and marginal distribution, $M/G/\infty$ Input model can simultaneously approximate autocorrelation function of real traffic. To do this, we use source lifetime distribution in form

$$\Pr\{\tau = k\} = \begin{cases} y, \ k = 1, \\ \frac{A}{(k+x)^{\alpha}}, \ k = 2, 3.. \end{cases}$$

instead of (1), x and y are fitting parameters. Using

$$y + \sum_{k=2}^{\infty} \frac{A}{(k+x)^{\alpha}} = 1$$

we get

$$A = \frac{1-y}{\sum_{k=2}^{\infty} (k+x)^{-\alpha}}$$

For normalized autocorrelation function of $M/G/\infty$ Input traffic (see for example [2])

$$r(k) = \frac{\sum_{i=k}^{\infty} \sum_{n=i+1}^{\infty} \Pr\{\tau = n\}}{y + \sum_{n=2}^{\infty} \Pr\{\tau = n\} + \sum_{i=1}^{\infty} \sum_{n=i+1}^{\infty} \Pr\{\tau = n\}}$$

After some transformations we get:

$$r(k) = \frac{(1-y)\sum_{i=k}^{\infty}\sum_{n=i+1}^{\infty}(n+x)^{-\alpha}}{\sum_{n=2}^{\infty}(n+x)^{-\alpha} + (1-y)\sum_{i=1}^{\infty}\sum_{n=i+1}^{\infty}(n+x)^{-\alpha}}$$

Using denotation \hat{r}_k for autocorrelation function of the real traffic trace, and performing minimization of

$$S(x,y) = \sum_{k=1}^{N} (r(k) - \hat{r}_k)^2$$

by *x* and *y*, we get this results.

In our experiments we made minimization by using MatLab.

Let us note, that after modification of lifetime distribution, it is necessary to reculculate λ .

Finally, autocorrelation function of simulated traffic is much close to real then before. (see on Figures 5).



Figure 5. Normalized autocorrelation functions for DEC-PKT-2.TCP trace rate

4. ON-OFF SOURCES MODEL

In opposite to previous model, here we assume, that there are M sources of traffic in the system and each of them has two possible states: ON and OFF. In OFF state the source

keeps silence, and in ON state it generates information flow. Each source switches between these states from time to time.

We consider the case, when each source during different ON periods can have different information rates. As before, rate for each new ON period are chosen at the beginning of the period and equal to realization of one of i.i.d. random values with generic integer random value ζ .

Durations of all ON periods of all sources are realizations of i.i.d. random values with generic integer random value τ , which has heavy tailed distribution (1). Again, α is calculated according to (2). As before, it provides second order asymptotical self-similarity of total traffic with given Hurst parameter. Durations of OFF periods of all sources are i.i.d with generic integer random value υ , which has geometric type distribution

$$\Pr\{\upsilon = k\} = p(1-p)^{k-1}, \quad k = 1, 2, \dots$$
(9)

where p is necessary to find.

4.1 ON-OFF version of source rate distribution calculation

From theory of alternating renewal processes stationary probabilities of each state for single source are given by



Figure 6. Traffic Distribution for BC-pAug89.TL trace

$$P_{ON} = \frac{E\tau}{E\tau + E\upsilon} = \frac{E\tau}{E\tau + 1/p} = \frac{pE\tau}{pE\tau + 1}$$
(10)

$$P_{OFF} = \frac{E\upsilon}{E\tau + E\upsilon} = \frac{1}{p\,E\tau + 1} \tag{11}$$

 $E\tau$ can be calculated numerically as before. Let us denote here p_i as probability to have *i* sources in ON state in some time slot. Independence of all sources gives, obviously, that

$$p_{i} = \binom{M}{i} P_{ON}^{i} P_{OFF}^{M-i}, \quad i = 0, 1, ... M$$
 (12)

No fictive sources condition gives, again, expression (5), and from (12) here we have

$$P_{OFF} = \sqrt[M]{\Pr\{Y_t = 0\}}$$
(13)

Using (11) and (13), we get value of p for distribution (9):

$$p = \frac{1}{E\tau} \left(\frac{1}{\sqrt[M]{\Pr\{Y_t = 0\}}} - 1 \right)$$
(14)

To get procedure for source rate distribution, we can follow exactly the same way as for $M/G/\infty$ Input model, with only one difference: number of sources now can not be more, then M. So, it is easy to see, that now expression (7) is valid only for $k \le M$ (where p_i are calculated by (12)). For k > M it must be

$$\Pr\{\zeta = k\} = \frac{\Pr\{Y_t = k\} - \sum_{m=2}^{M} p_m \Pr\left\{\sum_{n=1}^{m} \zeta_n = k\right\}}{p_1}$$
(15)



Figure 7. Source Rate Distribution for BC-pAug89.TL trace

4.2 Numerical results for ON-OFF sources model

Using H and $Pr{Y_t=k}$ from Ethernet traffic traces in equations (1), (2), (5), (9), (14), (15) for different values of M=2,...10 we found α , *p* and sequence of source rate probabilities $Pr{\zeta=k}$, and made the same numerical experiments for each M used, as for $M/G/\infty$ Input model. Then we choose the best M in terms of closest of real and simulated traffic distributions.

For both Ethernet traces the best M is 2. (It is necessary to note, that the best M is 1, obviously, but this case is trivial. This case does not give any inside in network behavior, it



just repeats traffic distribution as unique source distribution, therefore, we don't consider it.)

Figure 8. Traffic Distribution for BC-pOct89.TL trace



Figure 9. Source Rate Distribution for BC-pOct89.TL trace

The results for both models are shown on Figures 8, 9 and in Tables 3, 4. Source rates for both traces are shown on Figures 8 and 9.

Table 3. BC-pAug89.TL trace parameters comparison

Trace	Н	Average	Variance
Real	0,786	28,786	2158,722
Sim. M/G/∞	0,792	11,069	96,212
Sim ON- OFF	0,781	23,055	1315,212

Table 4. BC-pOct89.TL trace parameters comparison

Trace	Н	Average	Variance
Real	0,802	75,576	5948,424
Sim. M/G/∞	0,807	62,603	5286,218
Sim ON- OFF	0,789	71,755	6520,264

5. REMARKS AND CONCLUSIONS

Presented above results show that $M/G/\infty$ Input model works better for TCP traces then for Ethernet traces. The explanations of this fact can be different. One of possible explanation is follow: local network of large company usually consists of a few big segments connected to central cable by bridges. From central cable "point of view" these bridges are looked like main sources of traffic. Therefore On-Off sources model with small number of big sources is more adequate, then assumption about large number of small sources. But actual reason of this situation is still open problem.

Another problem is not very good accuracy in simulation of average and variance of real traffic. It is because algorithms presented here "pay most attention" to initial part of marginal distribution, but not to tail. But tail of distribution can affect much on first moments, especially on variance. So, some possible direction of future work is algorithms modification for more accurate simulation of marginal distribution tail. Another way to improve accuracy is more accurate estimation of $E\tau$. One possible such improvement was presented above. More accurate estimation of $E\tau$ of real traffic, for example, by estimation of initial part of autocorrelation function (see [2]), can improve accuracy of simulation marginal distribution and autocorrelation function simultaneously.

In conclusion we would like to note that models considered here is very useful for practice. For example, prediction by simulation of some growing organization network behavior can be made easily, if we take current organization traffic, find such parameters as λ (for M/G/ ∞ Input model) or *p* (for On-Off sources model), and increase it. In case of more complex analysis, it can be possible to identify the nature of individual source rate distribution in terms of mostly used network applications and make some prediction of this evolution.

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USING SIMULATION FOR DECISION MAKING IN ZERO LATENCY ENTERPRISE PROJECTS

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KEYWORDS

Distributed Simulation, High Level Architecture (HLA), Zero Latency Enterprise (ZLE).

ABSTRACT

The concept of Zero Latency Enterprise (ZLE) has received considerable attention through the last years. Many companies and organizations want to see the value of this kind of strategy before changing their IT infrastructure to implement ZLE solution. This paper proposes a new project methodology defining five main steps that should be followed to success in ZLE implementation projects. One of these steps, the Planning and Decision Making stage, is based on simulation techniques, allowing a comparison of the organization performance with and without ZLE strategies. Furthermore, in this work the different approaches for the ZLE simulation are examined and discussed.

INTRODUCTION

The competitiveness of current markets has lead many organizations to explore innovative strategies in order to enhance competitive differentiators. The Zero Latency Enterprise (ZLE) concept refers to a company in which business events recognized anywhere in the business can immediately trigger appropriate actions across the entire enterprise and beyond (White, 2001).

The ability to make decisions based on up-to-date information and to apply such decisions to reaction mechanisms clearly differentiates those companies that are capable of responding, acting, learning and adapting in real time (Ranavide, 1999).

Transforming an organization into a ZLE is a complex process that needs a detailed planning to achieve all the desired objectives with the required quality. The same data belonging to different applications and company departments use to be in different formats, to follow different rules and to be updated, modified and accessed through completely different processes. Therefore, ZLE projects are mainly related to integration and interoperability concepts.

The main contribution of this paper is the definition of a five steps methodology to implement ZLE strategies. One of the main problems during this implementation use to be the need of knowing the effects, costs, benefits and risks of this kind of strategy before making important decisions. ZLE implementation implies several challenges and difficulties and it is crucial for companies to know in advance the possible advantages and problems of the implementation.

This work proposes the use of simulation in the Decision Making step, providing a powerful mechanism to determine if ZLE is a profitable strategy for the company and to optimize its implementation if the project is finally carried out. Furthermore, a detailed analysis of the two main alternatives for this simulation, using monolithic or distributed models, are discussed to guide users in their ZLE projects.

The rest of this paper is organized as follows. Section 2 gives the theoretical background related t ZLE concepts and necessary to understand this work. Section 3 proposes the methodology for ZLE strategies implementation, and Section 4 analyzes the two main alternatives for simulation in the Decision Making step of the proposed methodology. Finally, Section 5, summarizes Conclusions and Future Work.

THEORETICAL BACKGROUND

Zero Latency Enterprise solutions allow applying real time concepts to business management. A ZLE strategy would be any strategy that exploits the immediate exchange of information across technical and organizational boundaries to achieve business benefit. ZLE describes organizations that can exchange information with employees, trading partners and customers in near real time, eliminating both internal and external latencies. In a ZLE organization, business events trigger system events that can post actions and send responses throughout the enterprise (Becker, 2001), (Hollar, 2003).

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) ZLE implies that the company has minimized the latency of their operations so that the events related to any factor affecting the company immediately trigger the timely actions of those responsible. The possibility of reacting in real time will bring to the company a competitive advantage.

Therefore we can summarize by saying that ZLE implies the minimization of business processes latency and allows information systems integration, bringing real time corporate information management.

The benefits of implementing a ZLE strategy can be summarized as follows:

- Provide a real time view of the business. The user will have all the information available in real time to react to problems as soon as possible.
- Detect and remove potential dangers and threats for the organization before they become a real problem.
- Increase productivity of business processes: achieve greater efficiencies, responsiveness and profitability.
- Access to applications available for real time business management (data mining, CRM, balance scorecard, business intelligence).

But despite all these advantages, the current corporate environments present several barriers and difficulties in implementing such strategies:

- Subsystems based on black boxes that cannot be accessed or modified to allow the desired integration.
- Lack of compatibility among software/hardware systems from different vendors and developers.
- Information islands existing in different abstraction or technological levels.
- Excessive business processes latency.
- Organization rejection and people negative attitude in facing new information systems and processes.
- Ignorance and/or mistrust in concepts relative to real time.

The ZLE approach can be deployed in any environment where real time information is required. But depending on the industry or sector (retail, financial services, telecommunications, etc), the applications and the functionalities will be different.

Focusing for example in the retail industry, these would be some of the applications and functions covered

by the ZLE approach: business intelligence, profitability forecasting, customer relationship management, supply chain management and marketing campaigns.

Technological Infrastructure for ZLE

One of the key factors necessary to implement a ZLE strategy is the software and network infrastructure that allows the systems integration, facilitates the business process latency reduction and provides real time information to corporate users.

The development and deployment of this infrastructure can be done from scratch or using some kind of software reengineering such as EAI. And the selected strategy can be based on a customized product, specifically developed for the organization; on EAI commercial solutions such as SeeBeyond or TIBCO; or on the infrastructure developed by Hewlett-Packard, the only ZLE software in the market nowadays (HP, 2009).

In any case, all these approaches are usually based on two technological concepts: Hub-and-Spoke and Web Services.

Hub-and-Spoke are applications composed of a central data integration repository and of a messaging services motor that allows communication through different applications. The Hub-and-Spoke is also responsible for carrying out the ETL (Extract, Transform and Load) tasks.

The most widespread definition of a Web Service is a software system designed to support interoperable machine-to-machine interaction over a network.

Web services are frequently just Web APIs that can be accessed over a network (LAN or WAN) and executed on remote systems. Therefore, Web Services are components accessible from different applications, and based in standard protocols. These components are loosely coupled and their basic unit of communication is the message.

IMPLEMENTING A ZERO LATENCY ENTER-PRISE STRATEGY

The implementation of a real time strategy will have an influence on almost all the divisions and departments within an organization, not only from a technological point of view (applications and data), but also from the viewpoint of innovation, processes or human resources, to name just some examples. The establishment of such a strategy requires a significant effort and in order to ensure success and a correct transition in the organization, a detailed methodology to develop the projects is needed. This work proposes a ZLE project roadmap composed of five different phases or stages:

- 1. Education and Communication.
- 2. State measurement and Benchmarking.
- 3. Information and Reporting.
- 4. Planning and Decision Making.
- 5. Implementation.

The first four stages should be always carried out in a ZLE project, but the fifth phase is performed only if in the Decision Making stage the cost/benefits analysis concludes that the ZLE strategy is a good option for the organization.

Next sections summarize these five stages proposed for the ZLE projects roadmap.

Education and Communication

The perception of the real time concept is often ambiguous or wrong. Two people talking about real time probably will talk about very different concepts. Therefore, for the success of the ZLE project, all the involved people must have a clear understanding, and more important, a common understanding of the concepts and technologies that are going to be handled.

This education is very important for other reasons, such as the involved departments' motivation, because without the cooperation and involvement of people working on the ZLE project, the achievement of the real time objectives will be impossible.

State measurement and Benchmarking

How prepared is the organization to ZLE?. To answer this question, all departments must examine in depth the current state of their IT infrastructures. This analysis will produce updated information about the qualitative and quantitative aspects that are important to the specific needs of the ZLE project. The state measurement can be performed within the organization or can be performed by external organizations or companies, in any case, an exhaustive benchmarking must be performed.

Information and Reporting

The data collected in the previous phase must be used to elaborate detailed information about the current organization applications, processes and information flows. Information about the available IT infrastructure and about the current organization resources must be elaborated too.

All this information must be reported to a ZLE project group responsible for performing the next step in the ZLE project roadmap: the Planning and Decision Making. Therefore, this group should be composed of people from all relevant departments and divisions of the organization.

Planning and Decision Making

After the reporting phase, the best ZLE strategy for the organization can be designed. In particular, the following aspects can be discerned: the processes and applications that will be needed to obtain a real time strategy, the departments necessarily involved in the ZLE strategy and the information flows between these departments.

Afterwards, a cost-benefit analysis must be performed to decide if it is profitable to carry out the project, taking into account the costs, the risks and the benefits of the ZLE implementation.

There are not analytical solutions for this evaluation because it is a too complex system, and qualitative aspects are not enough to take robust decisions because they not help in identifying the critical aspects for the project success.

A variety of simulation techniques have been previously applied to software development projects (Kellner et al., 1999). In this kind of work, simulation has demonstrated to be useful in predicting the costs and benefits of software projects (Donzelli and Iazeolla, 2001), (Host et al., 2001), (Raffo and Wakeland, 2003).

In this work simulation techniques are recommended as a tool to reach a decision in ZLE projects. A simulation of the performance of the company with and without ZLE can easily determine if it is a profitable strategy.

To improve decision making at this stage, simulation can be complemented with other techniques to determine more specific aspects, for example, about the low level technological details of the project or about specific applications.

But the simulation of the "virtual organization" should be the main decision mechanism on a project of this complexity. Furthermore, if it is decided to go ahead with the project, this simulation can really help in finding the optimal ZLE strategy for the organization.

These are the main questions that should be answered from simulation results:

- What would be the costs, benefits and risks associated with implementing ZLE?.
- How would the ZLE solution contribute to the company competitiveness?.
- What would be the impact of considering certain processes, applications or departments in the ZLE strategy?.

• What need to be done to ensure that the full benefits of ZLE are achieved?.

Implementation

If the Decision Making stage leads to the ZLE implementation, the old IT infrastructure is gradually replaced by the new, allowing real time. This transition must be a dynamic process in which the ZLE project group is responsible for avoiding unnecessary costs and latencies, and for ensuring that the specified quality is achieved and the project objectives are satisfied.

In a realistic environment, this implementation stage is almost always iterative, implementing the ZLE solution in small steps until the real-time objectives are met. In each of the iterations, the simulation can help to achieve the project goals faster and with less costs and risks.

ALTERNATIVES FOR THE SIMULATION IN THE DECISION MAKING STAGE

As it has been stated in the previous section, one of the most important steps in implementing a ZLE strategy is the simulation of the operation of the company before and after its implementation.

This stage allows estimating the costs and benefits involved in the ZLE project and making decisions not only with qualitative information. However, this stage can be expensive in time and resources, since it involves simulating the operation of different processes, applications and departments composing the organization, as well as information flows between them.

This may involve the simulation of models of manufacturing plants and infrastructures (production planning, flow of raw materials, resource consumption, production strategies), logistics and supply chain (suppliers behavior, demand, stocks) or different kind of business processes (business development, marketing, training).

In this section we analyze the two different approaches that can be used for this "virtual organization" simulation: the use of a monolithic model of the company created for the ZLE project or the use of a distributed simulation by exploiting the different models previously coded and used in the organization for other purposes.

Monolithic model

In this case, once the processes, systems and departments that are involved in the ZLE strategy are determined, a model of joint behavior of all of them is created from scratch to simulate their operation without and with ZLE.

To integrate into a single model so many heterogeneous subsystems, almost always it is necessary to create this model with a general purpose language such as Java, Fortran or C++. Only in certain simple cases COTS simulation packages such as Arena, Extend, FlexSim or Simul8 can be used to create the monolithic model for the Decision Making stage in the ZLE project roadmap.

Such a model can be very complex to obtain, and the modeler could greatly benefit from a design philosophy based on modularity, simplifying the process using libraries of re-usable modules. Although such libraries are common in the lower end of the simulation (mechanical and electrical systems or manufacturing processes, for example), unfortunately they are not yet widespread in the higher levels (business processes, for example). Therefore, it may be difficult to find pre-defined building blocks to model certain parts of the organization.

Documentation and execution of a single monolithic model are, in general, easy to perform. But this kind of model makes difficult the reuse of existing simulations; requires the people involved in the project to understand the low-level details of the company's operation; and the model updating whenever there is a change in the company will have a great cost. The disappearance, modification or addition of a subsystem in the organization make necessary to revise completely the monolithic model.

As a conclusion, this alternative is profitable only in small projects that either are located in small organizations, or involve only a small part of larger companies. The creation of a single monolithic model for more complex projects would be too expensive in time and resources, hard to maintain and furthermore, would reduce the quality of simulation results due to the simplifications that should be made to obtain it.

Distributed model

The use of simulation in business environments has become a *de facto standard*. When a company decides to deal with the implementation of a ZLE strategy, almost always exist in the organization models and simulators of different subsystems previously implemented.

The approach of distributed modelling tries to exploit these existing models in the company, but there are no tools to integrate heterogeneous models from arbitrary packages or programming languages automatically.

Building a distributed simulation is much more complex than building a monolithic model, since it involves many new concepts: integration of all models at run time, time synchronization, representation of the data to be exchanged, data and objects ownership management, etc. The simulation software used to model and predict the behavior of the manufacturing process or of the scheduling methodologies do not use the same data formats as the systems used to simulate the new products design or to re.-engineer the production system, for example. It can be very difficult to solve all these new problems, and if the modeler is not familiar with distributed simulation this difficulties can lead to semantic inconsistencies in the simulation. It is not enough to possess good knowledge in modelling and programming to complete a project of this type and the simulation results may suffer in terms of quality and performance.

The modelling phase is usually easy to perform because previously coded models can be used and if new models are needed, they can be coded separately, taking advantage of the best package or programming language for each subsystem and of building blocks libraries. But the documentation and execution are complicated, just the opposite of the monolithic model. A monolithic model simulation performs faster than a collection of coupled models, because there is no need for explicit time synchronization, for example.

Also unlike the monolithic model, the updating is much simpler, being the scalability one of the big advantages of distributed simulation.

When an organization needs to integrate different models, low-level technologies such as WinSock, COM or CORBA, have been traditionally used. But humans still play an important role in operating these systems and this kind of integration suffers from the typical disadvantages of customized solutions.

To overcome these limitations, a standard solution has been developed for distributed simulation: High Level Architecture (HLA). This standard was developed by the US Department of Defense in 1995 to solve the problem of distributed simulation by allowing different independent and heterogeneous models to interact in a federation (Morse et al., 2006).

A federated model can exchange data with the rest of models in the federation via a Run Time (RTI) implemented over a network in a time synchronized manner. This is achieved by separating the data model and architecture of the methods and functions used for the information exchange between models. The HLA specification consists of:

- HLA Framework and Rules (standard IEEE 1516): Define ten rules to specify the responsibilities of the federated simulators and federations to ensure a proper interaction between them.
- HLA Federate Interface Specification (standard IEEE 1516.1): Specifies the services and interfaces of the RTI (Runtime Infrastructure) that is used to communicate a federation, using a data network and tools for time synchronization between models.
- HLA Object Model Template (standard IEEE

1516.2): Provides the templates for the objects used to achieve interoperability between simulators, the Simulation Object Model (SOM) and the Federation Object Model (FOM).

Initially, there were only a few simulation projects in industrial environments in which the HLA standard was applied. This is mainly due to all the HLA features, important to military environments but not very useful for the industry simulation. These features add a great complexity to projects, unnecessarily, and the industry is not interested in technology but in obtaining results as quickly as possible and with as little investment as possible. Furthermore, the HLA specification presented certain ambiguities, making it difficult to integrate this standard with the typical COTS packages (Attila et al., 2006), (Attila et al., 2006), (Attila et al., 2008).

The main solution for these initial problems with HLA and industry has been the SISO CSPI PDG standard definition (Strassburger, 2006). It defines Interoperability Reference Models (IRM), to identify in a clear, simple and precise way the cases in which typical COTS packages should use HLA to federate two or more models in industrial environments. There are four types of IRM (Taylor et al., 2007):

- Type A: Entity transfer.
- Type B: Shared resource.
- Type C: Shared event.
- Type D: Shared data structure.

Their definition has enabled all COTS packages to build in HLA interfaces for distributed simulation, all of them integrating the HLA standard in the same way. Therefore, the federation of models encoded with COTS packages is much easier today thanks to the use of HLA and IRMs.

The difficulty is still in the integration of models coded with other packages or programming languages, due to lack of maturity of the HLA standard in industrial and business environments.

The evolution of technologies such as WebServices and of SOA programming philosophies (Banks et al., 2003) suggests that the future of distributed simulation will be in making simulations available through networks.

In the long term, an end user will be able to compose a federation through his browser, since the simulations of different models will reside in the LAN or WAN as web services. The latest versions of HLA already supports this kind of solution and there are a few works that go in this direction (Wu et al., 2007), (Zhang et al., 2008), but we are still far from achieving distributed simulations where the interoperability between heterogeneous models is transparent to the user to this point.

CONCLUSIONS AND FUTURE WORK

Today it is more crucial than ever for a company to be up to date and not miss time and/or resources in unnecessary latencies. This leads to a strong need of having business information in real time and to become a Zero Latency Enterprise.

The implementation of this kind of strategy use to involve many different processes, systems and departments of an organization, hence, ZLE projects must follow a clear an detailed methodology, considering both the costs and the benefits of the ZLE transition.

In this paper, a 5-steps methodology has been proposed, using simulation techniques in the 4th stage, Planning and Decision Making, to decide if the ZLE strategy implementation is profitable to the company. In authors' opinion, firms will not blindly adopt this kind of solution and will want to see its tangible benefits in the mean and long term. Therefore, simulation is a perfect solution for the Decision Making in ZLE projects, providing a robust tool to optimize the later ZLE strategy implementation.

The two main alternatives for the simulation stage have been examined in this work, discussing the advantages and drawbacks of using a monolithic and distributed models.

The bigger and more complex the project, the bigger the benefits from cutting it up into small subprojects. Distributed simulation reduces complexity by cutting things up into independent domains although it adds some new complexity introducing new concepts and problems that must be solved. HLA and IRMs can help to solve these aspects, but there is still a lot of work to do in this area.

Complexity and project size are, therefore, the main drivers to decide the best option for the simulation in the Decision Making stage of projects.

We are now working in the definition of new IRMs capable of defining typical situations in ZLE projects at a higher level than the IRMs currently available. A very interesting line for future research would be creating a library of re-usable models and simulation blocks with the more common models in ZLE projects. And exploring the possible solutions for making these models accessible from Internet to allow users composing distributed simulations through the network.

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AN APPLIED STEP IN FOREST FIRE SPREAD MODELLING

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KEYWORDS

Forest fire spread modelling, forest fire suppression, shape approach, cellular automata, crisis management, geographical information system.

ABSTRACT

We report in this paper on an experiment in implementing a fire spread modelling system specifically dedicated to fire-fighting activities. First, the corresponding operational framework is introduced. In particular, we stress the importance of time constraints. Then, forest fire modelling techniques as well as some considerations related to our experience and feedback on this issue are briefly tackled. Then, we bring in a model which appears as a mix between the shape approach and raster based models. This one involves both a raster representation of the landscape and an elliptical shape based approach. We conclude on the fact that the corresponding software system calculates fire contours which are correlated with actual ones provided the basic local rates of spread are accurately estimated.

INTRODUCTION

Forest fires periodically devastate forest ecosystems and often threaten local populations. Hence, huge means are usually deployed in order to fight this curse. In this setting, fire growth prediction is a key-concept for forest fire suppression management. Consequently, numerous research works are dedicated to this field. However, for the time being, many of the latter remain in the scope of the academic world. In fact, the leading operational systems are dedicated to North-American climates and vegetation. The adaptation of the latter outside the specific areas they have been designed for seems to be a difficult approach to implement. For the Mediterranean basin, several tools have been developed, e.g. CARDIN (Caballero et al., 1994), FOMFIS (Caballero et al., 1999), E-FIS (Caballero et al., 2001), Fire-station (Lopes et al., 2002), a Greek system presented in (Vakalis, 2004) and Firetactic (Intergraph, 2006).

In all cases, the elaboration of software systems used on the ground by fire-fighter units and with the ability to perform accurate forest fire simulations remains the ultimate goal. Thus, we wish to stress the fact that the applied work presented in this paper has been conducted in close relationship with fire-fighters. Thence, all along the project, the different technical choices have been motivated by a permanent concern of pragmatism.

THE OPERATIONAL FRAMEWORK

Forest fire suppression management

The work described in this paper is part of the Asphodèle project (Dumond, 2006) which brings together, since 2002, the University of Savoie and a fire brigade from the South of France. In this framework, our goal is the implementation of a software system dedicated to forest fire suppression management. Hence, the following are the main functionalities offered by this system:

- The elaboration of numerical battlefields (Figure 1) which synthesizes, along the intervention, the situation on the ground. Hence, fire contour(s), spreading axes, location of the different engaged means, the implemented strategy, etc. are drawn onto different kinds of background map, e.g. geological survey maps, aerial photographs, etc.



Figure 1: A numerical battlefield elaborated by means of the Asphodèle system © SDIS 06

- The management of all the mobile means involved in the fight, i.e. from the moment they have been requested up to the time they are relieved from their fighting duty. This implies a permanent contact between the officers who are at the head of the intervention and the units deployed on the ground. Moreover, the staff headquarters is periodically kept informed of the situation in the field.

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- Prospective activities, also called *anticipation*, which are directly related to fire growth and its potential consequences. These tasks are carried out by entrusted officers who are freed from the actual management of the intervention. Therefore, they can make accurate analyses in order to suggest evolutions in the implemented strategy. The reasonings carried out in this setting are based on careful study of the intervention zones by means of 3-D display and aerial photographs, as well as on numerical simulation. The contours of ancient fires which occurred in the same areas are also considered.

All the aforementioned tasks are achieved from two mobile command posts, i.e. heavy trucks specifically equipped for these purposes: one is the heart of the command line and the second hosts the anticipation tasks. In both cases, the corresponding embedded technology is made of several laptops with dedicated software and additional wide screens. Internet access through connection to the telephone network and radio communication are also provided.

Operational constraints related to anticipation

The anticipation tasks are strongly related to fire suppression management since part of their input data, e.g. fire contours, appear in numerical battlefields. What is more, they are generally performed in times of crisis with potential, if not actual, threats against population. This has at least two important consequences:

- A high level of inter-operability between the software components used to manage fighting activities and those implementing simulation is required.
- Numerical simulations must run efficiently on the available laptops. With respect to that issue, it is admitted that any simulation phase should not exceed a quarter of an hour: this clearly comes from the fact that any implementation of a new strategy on the ground requires a re-dispatching of the mobile means, which may take up to two hours.

The result furnished by an anticipation analysis is made of a digital battlefield including future estimated fire growth at a given term and the corresponding recommended strategy.

FOREST FIRE SPREAD MODELLING

Forest fire spread modelling is a multi-disciplinary field of research. Roughly speaking, it involves two kinds of work:

- Theoretical contributions which aim at elaborating physical models for forest fire spread. From a scientific point of view, this approach is clearly the most satisfying one insofar as it can potentially provide accurate results. However, it is generally hard, if not impossible, to put into practice for at least two reasons: first, it requires an amount of data which cannot generally be provided. For instance, if we consider models based on energy transfer, the precise quantity of burning fuel must be specified, which appears as an insurmountable problem with respect to the extreme heterogeneity of Mediterranean scrub. Second, these models are generally based on partial derivative equations systems which, at least for the moment, cannot be solved in realtime.

- Practical, i.e. statistical or semi-empirical, approaches which can be more easily implemented. Here, the corresponding models are partially the result of analytical works but also consist of the synthesis of numerous experiments, i.e. the corresponding formulae have been elaborated and validated empirically after the observation of actual forest fires (Martins Fernandes, 2001), (Dimitrakopoulos and Drita, 2003). Clearly, such pieces of information are strongly dependant on the setting they have been obtained in and therefore they generally cannot be used elsewhere. Among the tools related to models of this kind, the leading ones are the Prometheus system by the Forestry Canada Fire Danger Group (FCFDG, 1992) which has been accumulating data for several decades and the Behave (Rabner et al., 2001) and Farsite systems (Finney, 1998) from the United States Department of Agriculture which are based on the Rothermel's model (Rothermel, 1972).

Another important issue about fire spread modelling is the way the combined effect of wind and slope are taken into account. For many authors (Weise and Biging, 1997), (Viegas, 2004), these must be managed by means of a vectorial sum between the wind vector and an *equivalent-wind* slope vector. Note that this principle is the one that is applied in the Farsite system. Nevertheless, some studies, e.g. (Van Wagner, 1988), suggest that the influence of slope can be weighted through numerical coefficients that must be applied on the basic rates of spread. Based on experience, we have been led to the conclusion that the first approach is the right one.

At the end, let us mention that very good syntheses on forest fire spread modelling have been published in (Perry, 1998) and more recently in (Sullivan, 2007).

Shape based and raster based approaches

The software tools related to semi-empirical models are implemented either by means of a shape based or a raster based approach, e.g. cellular automata.

In the shape approach, fire contour is considered at time t. The local rate of spread is calculated for a given set of points belonging to the contour. Then, standard geometrical shapes, generally ellipses (Glasa and Halada, 2007) or double-ellipses, are drawn accordingly. At

this stage, the corresponding set of shapes defines the fire contour at time $t + \delta t$ (Figure 2).



Figure 2: Shape approach based on ellipses

In cellular-automata based approaches (Bodrozic et al., 2006), (Hernándes Encinas et al., 2007), and more generally in raster based ones (Green et al., 1990), (Vasconcelos and Guertin, 1992), the landscape is divided into a large number of cells. The corresponding grid is generally defined under the form of a 2-D array of square cells. Nevertheless, hexagonal cells (Trunfio, 2004) are sometimes employed. In such a framework, the relevance of the system essentially depends on the set rules that specify the conditions of fire propagation between cells. Furthermore, raster based software systems run faster than those based on shape approaches.

OUR EXPERIENCE FEEDBACK

In an earlier work (Dumond, 2007), we have implemented a software system for fire spread modelling. The latter was mainly dedicated to peri-urban areas characterized by a little accentuated relief. Thus, the salient features of this system were the following:

- We worked with the proviso that, in any case, fire would spread in the direction of local winds. Hence, the effect of slope was taken into account by means of numerical coefficients after (Van Wagner, 1988). In other words, we worked under the assumption of a pre-eminence of wind effect on slope effect.
- Fire spread modelling was implemented by means of a cellular automaton.

After experimentation in the field, we were led to two main conclusions. First, although main flame front locations were generally correlated with the reality, fire shapes were almost always too wide. Furthermore, the use of the system in hilly landscapes showed that our management of wind and slope effects was not suitable outside the scope the model was designed for. In fact, the influence of the slope was clearly under-estimated. For instance, the following phenomena were usually observed:

- Fire spreading uphill against an opposite wind due to steep slope.
- Fire spreading stopped on hill ridges whenever it faces an intense opposite wind (Figure 3).



Figure 3: Example of combined effect of wind and slope: here, fire spread is stopped on hill ridges © SDIS 83 - Groupement Est

Thus, it was clear that effects of wind and of slope can very well act against each other. In addition, the excessive breadth of fire contours was clearly due to orthogonal projections of the calculated rates of spread on the axes of the cellular automaton. These observations initiate the elaboration of a new model. Furthermore, we wished to take advantage of the relevance of the shape approach. This led us to the mixed model presented in this paper where the rates of spread along the different edges of a grid representing landscape are calculated by means of ellipses.

THE PROPOSED APPROACH

The available data

The following is the list of the data available for the calculation of fire growth:

- An altimetric database: a grid of square cells 50m x 50m is mapped onto the landscape. An altitude measure is assigned to each cell.
- A set of wind maps which provide the effect of the relief on the wind, thus providing local winds. The latter are specified by means of vectors, i.e. numerical data representing both intensity and direction *in 3-D* space. It is worth noting that these data can very notably vary between ridges and thalwegs (the latter are the lines defining the lowest points along the length of river beds or valleys). Again, the landscape is divided in cells, the dimensions of which are 50m x 50m. Also note that the two kinds of grid, i.e. altimetric database and wind maps, precisely overlap. Moreover, we have different maps which correspond to the set of all the different dominant winds, with various intensities, in the areas concerned.

- Vegetation maps which allow the definition of combustibility classes the landscape can be divided in.
- Furthermore, all the meteorological data, i.e. the direction and the intensity of the current wind, the temperature in the shade, the air moisture content, etc. are provided in real-time by the forecast service.

We specify hereafter the process of calculation of fire growth. Note that, in a first time, the problem is handled in a generic way, i.e. the different formulae actually used are specified later on in the paper.

Rate of spread calculation

Let us consider two cells C_1 and C_2 of the altimetric database. The calculation of the fire rate of spread from the centre of a burning cell A to that of a non-burning cell B involves the following steps:

First, note that the milieu (fuel characteristics, wind) is supposed to be homogeneous in the areas crossed respectively by the half-edges [A, H] and [H, B] (Figure 4). Hence, the calculation must be performed successively on the two half-edges. Hereafter, we treat the case of the first one, i.e. [A, H]. Let S be the "equivalent-wind" slope vector between the points A and H: S is at the vertical of [A, H] and its orientation is defined with the proviso that on the ground, the altitude of the point H is superior to that of A: the value of the angle α is given as a function of this difference.



Figure 4: Slope vector \vec{S} w.r.t. the edge [A, H]

- Let \vec{W} be the wind vector in the cell C_1 . Thus, the calculation described hereafter can very well be performed in the plane defined by the two vectors \vec{S} and \vec{W} (Figure 5). Thus, the vectorial sum $\vec{C} = \vec{W} + \vec{S}$ specifies the combined effect of wind and slope on the fire spread on the ground at the vertical of the edge [A, H]. In the present setting, we do not regard opposed-wind fire spread as a credible hypothesis. Hence, if the value of the angle made by the vectors \vec{S} and \vec{C} exceeds $\frac{\pi}{2}$, then fire spread is considered as impossible on the edge [A, H]. Otherwise, by application of a given formula, e.g. the one given at the next section, we calculate the norm of the basic rate of spread vector \vec{B} on the axis specified by the vector \vec{C} . The norm in question is generally defined as a function of the norm of \vec{C} as well as the kind of vegetation and some physical parameters, e.g. air, soil and vegetation water content, temperature, sun exposure, etc.

At this stage, we can apply to the present setting the elliptic shape hypothesis (Richards, 2005), (Glasa and Halada, 2007). Hence, the shape of local fire is assumed to be represented under the form of an ellipse, the rear focus of which being the ignition point. Hence, we consider that, once it has been calculated, the norm $|\vec{B}|$ of the basic rate of spread vector defines the distance between the rear focus of the ellipse, located at the point *A*, and the opposite extremity of the latter. Note that the ellipse's eccentricity is provided by a formula as a function of the norm of the wind-slope resultant vector.

Then, the norm of the vector \vec{R} , i.e. the fire rate of spread on the ground at the vertical of the edge [A, H], is provided by a radial projection according to the defined ellipse (Figure 5):



Figure 5: Calculation of the norm of the vector \vec{R} by means of a radial projection according to an ellipse.

- At the end, the rate of spread vector \vec{R}_s along the edge [A, H], i.e. on the underlying 2-D grid, is obtained by an orthogonal projection of \vec{R} on the line defined by the points A and H (Figure 6):



Figure 6: Calculation of the rate of spread \vec{R}_s along the edge [A, H]

The above calculation process deserves the following comments:

- First, it must be repeated for all the edges on which the fire rate of spread have to be calculated. On flat land, i.e. if $\vec{S} = \vec{0}$, and in an homogenous milieu, it leads to an elliptic shape under the assumption of a constant wind, and to a circle in case of absence of wind.
- The sense (always bottom-up) of the slope vector \vec{S} is given by the relative altitudes associated to the two points considered, here *A* and *H*.

- The above approach can easily be generalized to any edge crossing a given cell: this makes possible to consider fire spread between non-adjacent cells. Hence, the altitude of the points defining the different edges concerned must be calculated by interpolation. Thus, in the algorithm given below, fire spread from a burning cell is potentially considered in the direction of 16 different cells, 8 of them being in the immediate neighbourhood of the initial cell and 8 being beyond (Figure 7):



Figure 7: Fire spread in 16 potential directions

Fire spread calculation

The conditions of fire spread from a cell to another being specified, the overall algorithm is fairly simple. Thus, we start from a set of burning cells which belong to one or several fire contours. Then, for each of these ones, we discriminate over the 16 potential targets, the cells which are not already burning. Then, we calculate the corresponding rates of spread and consequently the spread durations respectively associated to each edge concerned.

Thus, when this task has been completed, the set of cells that are in a position to be fired by the burning cells has been elaborated. This one is hereafter referred to as the *fire vicinity*. At this stage, we select in the fire vicinity, the cell associated to the shortest edge, in terms of duration: the latter will be the next one to be reached by the fire. Thence, once the durations respectively associated to the corresponding edges have been calculated, the cell in question is replaced in the fire vicinity by those which are its potential targets. This iterative process is stopped when the deadline, i.e. the lapse of time considered in the simulation, expires.

Implementation

We provide hereafter some pieces of information related to the implementation of the above specified approach:

- The norm of the slope vector is given by a formula which provides an "equivalent-wind" value as a function of the angle α of the considered edge with the horizontal. For instance, the formula given in (Lopes et al., 2002) is:

$$|\vec{S}| = 15.275 * \beta^{-0.0225} * (tan(\alpha))^2$$
 (1)

where:

- α is the slope.
- β is a parameter which depends on the fuel bed.
- *tan* is the tangent function,

Based on our experience, the formula $12 * (tan(\alpha))^2$ is suitable for the heterogeneous Mediterranean scrub. In particular, it provides an equivalent-wind speed of $12 m s^{-1}$ for a slope of 45 degrees.

- The norm of the basic rate of spread vector $|\vec{B}|$ is obtained by means of the Drouet's formula (unpublished work):

$$|\vec{B}| = 180 * e^{0.06*T_s} * tanh(\frac{100-S_w}{150}) *(1+2*(0.8483+tanh(\frac{|\vec{C}|}{30}-1.25)))$$
(2)

where:

- T_s is the temperature in the shade, given in Celsius degrees.
- *S_w* is the soil water content, expressed in millimeters.
- $|\vec{C}|$ is the norm of the wind-slope vector, given in kilometers per hour.
- *tanh* is the hyperbolic tangent function.

Note that although this formula has been designed for the Mediterranean zone, it does not deal with vegetation and air moisture content which is an actual shortcoming. Hence, we have to take into account the nature of the vegetation by means of numerical coefficients. Moreover, a study of the influence of air moisture content on fire rate of spread is in progress at the present time.

- The equation of an ellipse in polar coordinates, with one focus at the origin, has the following form:

$$\rho = \frac{p}{1 + e * \cos(\alpha)} \tag{3}$$

where p and e are respectively the parameter and the eccentricity of the ellipse. The latter can be expressed as a function of the length to width ratio $\frac{L}{W}$ of the ellipse:

$$e = \sqrt{1 - \frac{1}{\left(\frac{L}{W}\right)^2}} \tag{4}$$

Thence, by considering the case $\alpha = 0$, we can deduce that the parameter of the ellipse is given by

$$p = (1+e) * |\vec{B}| = (1 + \sqrt{1 - \frac{1}{(\frac{L}{W})^2}}) * |\vec{B}| \quad (5)$$

What is more, some authors provide an estimation of the $\frac{L}{W}$ ratio as a function of the norm of the windslope vector $|\vec{C}|$. For instance, the following is the formula given in (Alexander, 1985):

$$\frac{L}{W} = 1 + 0.0012 * (2.237 * |\vec{C}|)^{2.154}$$
(6)

Note that in our setting, this ratio has to be doubled in order to provide realistic fire shapes.

Thus, the data e and p being determined, if θ is the angle between the vectors \vec{C} and \vec{R} , the norm of the latter can be immediately deduced from equation (3):

$$|\vec{R}| = \frac{p}{1 + e * \cos(\theta)} \tag{7}$$

- The system has been developed in a C++ programming environment and runs under Windows XP. Furthermore, data are provided by the *GeoConcept* geographical information system.

We provide hereafter (Figure 8) an example of simulation performed with the system presented in this paper. This fire directly threatened the suburbs of the city of Cannes (South France) during the night from the 5th to the 6th of July 2007.



Figure 8: Result of a simulation © SDIS 06

Comments on Figure 8:

- The ignition time was 5 p.m.
- The burned area at 10 p.m. is represented in blue.
- The flame front at 10 p.m. is represented in red.
- The successive fire contours, separated by a time interval of one hour, i.e. from 10 p.m. up to 3 a.m., are represented by means of the different orange lines.
- The burned surface is around 450 hectares. The fire travelled around 7 km in 10 hours, which is an average rate of spread in the framework concerned.
- The simulation given below was obtained in less than three minutes on an Intel Core Duo based laptop with four Giga-bytes RAM.

CONCLUSION

The forest fire spread model presented in this paper takes into account the three following concepts:

- Geographical information that aims to faithfully represent the characteristics of the areas concerned.
- Physical models that make possible the calculation, by means of given set of formulae, of the different local rates of spread as a function of the various available physical and geographical parameters.

- An algorithm that manages fire spread.

At this stage of our work, we can draw the following conclusions:

- Whenever the Drouet's formula provides reliable data, i.e. if calculated basic rates of spread match the measurements taken on the ground, the actual fire shapes are correlated with those resulting from simulation.
- Important differences between the results of the application of the Drouet's formula and actual rates of spread are noted when air moisture content is extremely low.
- Due to the simplicity of the fire spread model, the system fits the operational timing constraints of the setting we are dealing with. Moreover, it offers a high level of inter-operability with the other software components.

Furthermore, the fire spread model will be subject to the following additional works:

- The elaboration of new formulae for basic rate of spread calculation. These ones will have to take into account supplementary data such as vegetation cover and air moisture content.
- Integration of additional geographic data, e.g. cliffs, non-flammable areas, etc. which have a huge influence on fire spread.
- Management of potential fire-fighters actions, e.g. front lines, side attacks, retardant droppings, etc. in order to evaluate the results obtained in the framework of various prospective scenarios.

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INVESTIGATING THE IMPACT OF INFORMATION SHARING IN A TWO-LEVEL SUPPLY CHAIN USING BUSINESS PROCESS MODELING AND SIMULATIONS: A CASE STUDY

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KEYWORDS

Supply chain, information sharing, business processes modelling, simulation, bullwhip effect

ABSTRACT

This paper reports on an oil/retail petrol supply chain which was undergoing a Business Process Reengineering (BPR) exercise. The paper models and analyses the effect of information sharing on the performance parameters (inventory costs and bullwhip effect) of an actual Serbian oil industry supply chain. The main idea is to show through business process modelling how the BPR of existing processes needs to follow the introduction of the EDI system into organisations to improve information sharing between the supply chain echelons. Also, a simulation is employed to show how different levels of information sharing impact on inventory costs and the bullwhip effect. The model itself was has developed for a twolevel supply chain structure, and it and its associated simulations highlight the significant benefits that are achievable through the use of improved information sharing and business process re-engineering on the observed supply chain performance parameters.

1. INTRODUCTION

Global marketplaces, higher levels of product variety, shorter product life cycles, and demand for a premium customer service are increasing supply chain complexity and cost. This coupled with advances in information technology are enabling companies to critically re-evaluate and improve their supply chain strategies and explore new modes for management supply chain activity. The supply chain, as a network of suppliers, factories, distribution centres and retailers through which materials are required, transformed and delivered to customers, often encounters the conflicting objectives of its members. Yet for success of the global optimisation of a supply chain collaboration between the different companies is vital. However, supply chain collaboration is only possible if supply chain partners share their information. It is well recognised that advances in information technologies have driven much change through supply chain and logistics management services. Traditionally, the management of information has been somewhat neglected. The method of information transferring carried out by members of the supply chain has consisted of placing orders with the member directly above them. This has caused many problems in the supply chain. These include excessive inventory holding, longer lead times and reduced service levels in addition to increased demand variability or the 'Bullwhip Effect' (BWE). Thus, as supply chain management (SCM) progresses, supply chain managers are realising the need to utilise improved information sharing throughout the supply chain in order to remain competitive.

However, the simple use of information technology (IT) applications to improve information transfers between supply chain members is not in itself enough to realise the benefits of information sharing. A mere increase in information transfers does not mean that information distortions (BWE) will be avoiding and the efficiency of logistics processes will be improving. The business models of existing processes have to be changed so as to facilitate the better use of the information transferred (Trkman et al. 2007). In this paper, by using business processes modelling and simulation we show how achieving only successful business process changes can contribute to the full utilisation of improved information sharing in supply chains. We analyse a two-level supply chain similar to that in (Trkman et al. 2007). There is a single supplier which supplies products to a retailer who, in turn, faces demands from end-customers. In this paper, we consider two information sharing strategies combined with three business process models, and two inventory control strategies that were being examined by the case-study company. In order to model the situation in detail, a discrete events simulation model of the supply chain has been developed. One aim of this study is to connect existing theoretical studies with a real-life complex case study in an attempt to provide people in the work world with the expected performance improvements discussed in this paper.

The next section briefly reviews related literature about the key concepts of the chosen topic. Section 3 formulates the case study and outlines business process models for the current and proposed state for the company under consideration. Section 4 details a

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) simulation study with experimentation concerning information sharing, business process models and a type of inventory control, while Section 5 discusses the results and concludes.

2. SUPPLY CHAIN MANAGEMENT

The objective of supply chain management is to provide a high velocity flow of high quality, relevant information that enables suppliers to provide for the uninterrupted and precisely timed flow of materials to excellence customers. Supply chain requires standardised business processes supported by a comprehensive data foundation, advanced information technology support and highly capable personnel. It needs to ensure that all supply chain practitioners' actions are directed at extracting maximum value. According to (Simchi-Levi et al. 2003), supply chain management represents the process of planning, implementing and controlling the efficient, costeffective flow and storage of raw materials, in-process inventory, finished goods, and related information from the point of origin to the point of consumption for the purpose of meeting customers' requirements.

2.1 Information sharing

In traditional supply chains, retailers make their own inventory replenishment decision based on their demand forecast and their cost structure. Many supply chain related problems such as BWE can be attributed to a lack of information sharing among various members in the supply chain. Sharing information has been recognised as an effective approach to reducing demand distortion and improving supply chain performance (Lee et al. 1997a). Accordingly, the primary benefit of sharing demand and inventory information is a reduction in the BWE and, hence, a reduction in inventory holding and shortage costs within the supply chain. The value of information sharing within a supply chain has been extensively analysed by researches. Various studies have used a simulation to evaluate the value of information sharing in supply chains (Towill et al. 1992; Bourland et al. 1996; Chen 1998; Gavirneni et al. 1999; Dejonckheere et al. 2004; Ferguson and Ketzenberg 2006). Detailed information about the amount and type of information sharing can be found in (Li et al. 2005).

The existing literature has investigated the value of information sharing as a consequence of implementing modern information technology. However, the formation of a business model and utilisation of information is also crucial. Information should be readily available to all companies in supply chains and the business processes should be structured so as to allow the full use of this information (Trkman et al. 2007). The objective of this paper is to offer insights into how the value of information sharing within a twolevel supply chain is affected when two different models of business process re-engineering are applied. Moreover, the literature shows that, although numerous studies have been carried out to determine the value of information sharing, little has been published on real systems. The results in this paper have been obtained through a study of a real-life supply chain case study using simulation.

2.2 The bullwhip effect

Our study has two objectives. First, as mentioned above, to investigate the impact of business process reengineering on information sharing value, as measured by lead times and transactional costs. Second, to examine the impact of information sharing with combinations of different inventory control policies on BWE and inventory holding costs.

An important observation in supply chain management is the BWE. Basically, this effect illustrates an increase in demand variability as one moves up the supply chain, i.e., from the retailer to the supplier. In order to effectively manage the BWE its primary causes must be understood. The main causes of the BWE were identified in (Lee et al. 1997a; Lee et al. 1997b) where solutions to manage it to were also offered. They logically and mathematically proved that the key causes of the BWE are: demand forecasting updating, order batching, price fluctuation, and shortage gaming. According to this researcher, the key to managing the BWE is to share information with other members of the supply chain. In these papers, they also highlighted the key techniques to manage the BWE.

We can measure the BWE in different ways, but for the purpose of this research we accepted the measures applied in (Fransoo and Wouters 2000). We measure the BWE as the quotient of the coefficient of variation of demand generated by one echelon(s) and the coefficient of variation of demand received by this echelon:

where

$$c_{out} = \frac{\sigma(D_{out}(t, t+T))}{\mu(D_{out}(t, t+T))}$$
(2)

(1)

 $w = \frac{C_{out}}{C_{in}}$

and

$$c_{in} = \frac{\sigma(D_{in}(t, t+T))}{\mu(D_{in}(t, t+T))}$$
(3)

 $D_{out}(t,t+T)$ and $D_{in}(t,t+T)$ are the demands during time interval (t, t+T). For detailed information about measurement issues, see (Fransoo and Wouters 2000).

2.3 Business process modelling

The business process is a set of related activities which make some value by transforming some inputs into valuable outputs. A business process model is an abstraction of a business that shows how business components are related to each other and how they operate. Its ultimate purpose is to provide a clear picture of the enterprise's current state and to determine its vision for the future. Modelling a complex business requires the application of multiple views. Each view is a simplified description (an abstraction) of a business from a particular perspective or vantage point, covering particular concerns and omitting entities not relevant to this perspective. To describe a specific business view process mapping is used. It consists of tools that enable us to document, analyse, improve, streamline, and redesign the way the company performs its work. Process mapping provides a critical assessment of what really happens inside a given company. The usual goal is to define two process states: AS-IS and TO-BE. The AS-IS state defines how a company's work is currently being performed. The TO-BE state defines the optimal performance level of "AS-IS". In other words, to streamline the existing process and remove all rework, delays, bottlenecks and assignable causes of variation, there is a need to achieve the TO-BE state. Business process modelling and the evaluation of different alternative scenarios (TO-BE models) for improvement by simulation are usually the driving factors of the business renovation process (Bosilj-Vuksic et al. 2002). In the next section a detailed case study of a Serbian petrol company is presented.

3. CASE STUDY: BUSINESS PROCESS RE-ENGINEERING

The case study is a Serbian oil downstream company. Its sales and distribution cover the full range of petroleum products for the domestic market: petrol stations, retail and industries. The enterprise supply chain comprises fuel depot-terminals (distribution centre), petrol stations and final customers. The products are distributed using tank tracks. The majority of deliveries is accomplished with own trucks, and a small percentage of these trucks is hired. The region for distribution is northern Serbia. It is covered by two distribution centres and many petrol stations at different locations. In line with the aim of the paper only a fragment, namely the procurement process, will be shown in the next section. A broader description of the case study can be found in (Maslaric 2008).

From the supply chain point of view, the oil industry is a specific business, and for many reasons it is still generally based on the traditional model. The product is manufactured, marketed, sold and distributed to customers. In other industries, advanced supply chain operation is becoming increasingly driven by demandpull requirements from the customer. There is a strong vertically integrated nature of oil companies and that may be a potential advantage. In other industries, much attention is focused on value chain integration across multiple manufacturers, suppliers and customers. In the oil industry, more links in the chain are "in house", suggesting simpler integration. In practice, there is still a long way to go to achieve full integration in the oil supply chain.

3.1 AS-IS model development

The next section covers the modelling of the existing situation (AS-IS) in the procurement process of the observed downstream supply chain case study. The objective was to map out in a structured way the distribution processes of the oil company. The modelling tools used in this case study come from the Igrafx Process. These modelling tools were applied in order to identify the sequence of distribution activities, as well as the decisions to be taken in various steps of the distribution processes. The AS-IS model was initially designed so that the personnel involved in the distribution processes could review them, and after that the final model shown in Figure 1 was developed.

The core objective of supply chains is to deliver the right product at the right time, at the right price and safely. In a highly competitive market, each aims to carry this out more effectively, more efficiently and more profitably than the competitors. Because both the prices and quality of petrol in Europe are regulated, the main quality indicator in oil supply chains is the number of stock-outs. The main cost drivers are therefore: number of stock-outs, stock level at the petrol station and process execution costs. Lead time is defined as the time between the start (measurement of the stock level) and the end (either the arrival at a petrol station or the decision not to place an order) of the process (Trkman et al. 2007).

The main problems identified when analysing the AS-IS model relate to the company's performance according to local optimisation instead of global optimisation. The silo mentality is identified as a prime constraint in the observed case study. Other problems are in inefficient and costly information transfer mainly due to the application of poor information technology. There is no optimisation of the performance of the supply chain as a whole. Purchasing, transport and shipping are all run by people managing local, individual operations. They have targets, incentives and local operational pressures. Everything was being done at the level of the functional silo despite the definition that local optimisation leads to global deterioration. The full list of problems identified on tactical and strategic levels are identical to those in (Trkman et al. 2007), so for greater detail see that paper.

Based on the mentioned problems, some improvements are proposed. The main changes lie in improved integration of whole parts of the supply chain and centralised distribution process management.

3.2 Business processes re-engineering

The emphasis in business process re-engineering is put on changing how information transfers are achieved. A necessary, but no means sufficient condition for this is to implement new information technologies which enable efficient and cheap information transfers. Hence, IT support is not enough as deep structural and organisational changes are needed to fully realise the potential benefits of applying new IT. In this case study we develop two different propositions for business process re-engineering (two TO-BE models) to show how the implementation of new IT without business process renovation and the related organisational changes does not mean the full optimisation of supply chain performance. The first renewed business model (TO-BE 1) is shown in Figure 2 and represents the case of implementing IT without structural changes to business processes. In the TO-BE 1 model, there is no integrated and co-ordinated activity through the supply chain. Inventory management at the petrol stations and distribution centre is still not co-ordinated.



Figure 1: AS IS model of the process

The TO-BE 2 model assumes that the processes in the whole downstream oil supply chain are full integrated and the distribution centre takes responsibility for the whole procurement process. The TO-BE 2 business model is shown in Figure 3. The main idea is that a new organisational unit within the distribution centre takes on a strategic role in co-ordinating inventory management and in providing a sufficient inventory level at the petrol stations and distribution centre to fulfil the demand of the end customer. It takes all the important decisions regarding orders in order to realise this goal. Other changes proposed in the TO-BE 2 model are the automatic measurement of petrol levels at petrol stations and the automatic transfer of such data to the central unit responsible for petrol replenishment; the

predicting of future demand by using progressive tools; and using operations research methods to optimise the transportation paths and times. The role of IT in all of these suggestions is crucial.

3.3 Measuring the effect of re-engineering

The effect of the changes can be estimated through simulations. Because our study has two objectives, we have two kind of simulations. In our first example we simulated business processes to investigate the impact of business process re-engineering on the information sharing value, measured by lead times and transactional costs. The second simulation, which partly uses the results of the first simulation, represents an objectoriented simulation which helps define the impact of information sharing and appropriate inventory control on the BWE and inventory holding costs in the oil downstream supply chain under consideration. Both simulations are especially important as they enable us to estimate the consequence of possible experiments. In the first simulation we estimated changes in process execution costs and lead times. First a three-month simulation of the AS-IS and of both the TO-BE models was run.



Figure 2: TO-BE 1 model of the process



Figure 3: TO-BE 2 model of the process

In the AS-IS model a new transaction is generated daily (the level of petrol is checked once a day), in the TO-BE it is generated on an hourly basis (the level of stock is checked automatically every hour). The convincing results are summarised in Table 1. The label "Yes" refers to those transactions that lead to the order and delivery of petrol, while the label "No" means a transaction where an order was not made since the petrol level was sufficient.

Table 1: C	omparison of	simulation	results for	or the A	S-IS a	and TO-	BE models

Transaction	No.	Av. lead time (hrs)	Av. work (hrs)	Av. wait (hrs)	Average costs (€)
Yes (AS-IS)	46	33.60	11.67	21.93	60.10
No (AS-IS)	17	8.43	2.40	6.03	8.47
Yes (TO-BE 1)	46	27.22	10.26	16.96	56.74
No (TO-BE 1)	1489	0.00	0.00	0.00	0.00
Yes (TO-BE 2)	46	12.85	4.88	7.98	32.54
No (TO-BE 2)	1489	0.00	0.00	0.00	0.00

The average process costs are reduced by almost 50%, while the average lead time is cut by 62% in the case of the TO-BE 2 business model. From this it is clear that this renovation project is justifiable from the cost and time perspectives. The results in Table 2 show that a full improvement in supply chain performances is only possible in the case of implementing both IT which enables efficient information sharing and the redesign of business processes. The mere implementing of IT without structural and organisational changes in business processes would not contribute to realising the full benefit.

The results of the previous simulation (lead time) were used as an input for the next simulation so as to help us find the impact of information sharing on the BWE and inventory holding costs in the given supply chain.

4. INVENTORY CONTROL SIMULATION

In this section we employed an object-oriented simulation to quantify the benefit of information sharing in the case study. The system in our case study is a discrete one since supply chain activities, such as order fulfilment, inventory replenishment and product delivery, are triggered by customers' orders. These activities can therefore be viewed as discrete events. A three-month simulation of the level of stock at a petrol station that is open 24 hours per day was run.

In order to provide results for the observed supply chain performance, the following parameters are set:

- *Demand pattern*: Historical demand from the endcustomer to petrol stations, and from petrol stations to distribution centres was studied. From this historical demand, a probability distribution was created.
- *Forecasting models*: The exponential smoothing method was used to forecast future demand.
- Information sharing: Two different types of information sharing were considered: (1) NoIS no information sharing (AS-IS model); and (2) IS
 Full information sharing (TO-BE models).
- *Lead time*: Lead time from the previous simulation business process was used.

- Inventory control: Three types of inventory replenishment policy were used: (1) No inventory policy based on logistics principles. There was a current state in the viewed supply chain (AS-IS model; (2) The petrol station and distribution centre implement the (R,Q) inventory policy according to demand information from the endcustomer, but the distribution centre was not responsible for the petrol station's replenishment policy – no VMI policy (TO-BE 1 model); and (3) VMI - full information sharing is adopted and the distribution centre is in charge of the inventory control of the petrol station. The one central unit for inventory control determines the time for replenishment as well as the quantities of replenishment (TO-BE 2 model).
- *Inventory cost*: This is the cost of holding stocks for one period.
- *Bullwhip effect*: The value of the BWE is measured from equations (1), (2) and (3).

To investigate the effect of information sharing upon supply chain performance (BWE and inventory costs), three scenarios are designed with respect to the above parameters:

- Scenario 1: No IS, no defined inventory control, (AS-IS model);
- Scenario 2: IS, no VMI, (TO-BE 1) model; and
- Scenario 3: IS, VMI, (TO-BE 2) model.

The simulation was run using GoldSim Pro 9.0. The results from Figure 4 show that the value of the BWE is smallest for Scenario 3, which assumed full information sharing with appropriate structural changes of business processes, and full co-ordination in inventory control across the supply chain. These results also show that fully utilising the benefit of implementing IT and inventory management based on logistics principles can decrease the BWE by 28% in the observed case study. In Figure 5 a comparison of inventory costs with regard to the scenarios is shown. The minimum inventory holding costs are seen in Scenario 3, like in the first case. The results from Figure 5 show that benefits from the application of new IT, business process reengineering and co-ordinated inventory policy,

expressed by decreasing inventory holding costs, could be 20%.



Figure 4: BWE value comparison of the three scenarios



Figure 5: Inventory costs comparison of the three scenarios

5. CONCLUSION

SCM has become a powerful tool for facing up to the challenge of global business competition because SCM can significantly improve supply chain performance. This paper explores the effect of information sharing with regard to the performance of a two-level oil downstream supply chain. The conclusions of the simulation experiments are: information sharing can enhance the performance of the supply chain. In addition, business process re-engineering, co-ordination and collaboration are also important mechanisms in the supply chain to improve performance. Collaboration can reduce the influence of the Bullwhip effect and improve cost efficiency.

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MODELING OF OXYGEN EFFECT ON KINETICS OF BATCH FERMENTATION PROCESS FOR YOGURT STARTER CULTURE FORMATION

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KEYWORDS

Mathematical modeling, fermentation kinetics, protocooperation, yogurt starter culture.

ABSTRACT

The aim of this work is to describe the kinetics of yogurt starter culture production by *S.thermophilus* 13a and *Lb. bulgaricus* 2-11 and to quantitatively analyse the effect of different dissolved oxygen concentration in the milk on the process trend. Five different mathematical models for description of process kinetics are tested and the best one is selected. The increase of initial concentration of dissolved oxygen leads to a proportional decrease in the specific growth rate of the population and of the rates of lactose consumption and lactic acid production. On the basis of this investigations, two zones of initial dissolved oxygen concentration are defined. In each of these zones, the associated pair of microorganisms have different behaviour.

INTRODUCTION

The interaction between *Streptococcus thermophilus* and *Lactobacillus bulgaricus* in a yogurt starter culture is characterized with an ecological indication named proto-cooperation [Driessen 1987, Simova et al. 1999]. The proto-cooperation is a basis for the symbiotic relationship build up between two species and collaborative metabolism with positive effect on fermented milk. The symbiotic co-existence of the

selected strains *S.thermophilus* and *Lb. bulgaricus* determines the typicality and strict individuality of yogurt. These two microorganisms that mutually provide for their development modify milk composition and as a result a product with specific nutritional profile is obtained. Furthermore, the microorganisms produce the specific aroma-defining compounds that in combination with other metabolites lead to specific aroma of the target product. The creation of a stable symbiotic association between a *S.thermophilus* and *Lb. bulgaricus* is really hard and time consuming process sometimes with no result [Driessen 1987, Driessen et al 1982a, Tamime and Robinson 2003].

Contributions of each of two micro organisms for such an interaction are investigated and some basic elements of mutual growth of lactobacillus and streptococcus are defined [Driessen 1987, Radke-Michell and Sandine 1986, Driessen et al. 1982a, Driessen et al. 1982b, Amoroso and Nanca de Nandra 1990, Farrow and Collins, 1984; Louaileche et al. 1993, Marshall, 1987, Radke-Michell and Sandine 1984,Tammam et al. 2000, Thunell and Sandine 1985, Tinson et al. 1982, Zourari et al. 1992]. The allegation that carbon dioxide is the unique element of proto-cooperation [Driessen et al. 1982b] has no scientific explanation by now. There is no proof that CO_2 takes part in *Lb. bulgaricus* metabolism too.

In answer to the question which is the stimulating factor for *Lb. bulgaricus* in the case of low urea activity of its partner in the associate pair, a detailed investigation of the specific role of milk dissolved oxygen in thermophilic

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) streptococcus and lactobacillus metabolism is carried out [Simova et al. 1999, Simova and Beshkova 2007, Simova 2007]. It is proven that the oxygen-tolerance of *S.thermophilus* 13a is the main growth factor for both investigated species in the starter culture as well as the main factor for proto-cooperation between them. *S.thermophilus* 13a assimilates oxygen in milk very quickly and in this way assures the anaerobic conditions required by *Lb. bulgaricus* 2-11. The Lactobacillus is actively cultivated and stimulates the metabolism of the mixed culture [Simova et al. 1999, Simova and Beshkova 2007, Angelov et al. 2002, Simova 2002, Simova 2007].

The main purpose of this work is to describe the kinetics of a yogurt starter culture consisting of *S.thermophilus* 13a and *Lb. bulgaricus* 2-11, using the investigation methods mentioned above, and to quantitatively analyse the effect of different oxygen concentrations on the starter culture formation.

MICROORGANISMS AND CULTIVATION CONDITIONS

Natural strains *S.thermophilus* 13a and *Lb. bulgaricus* 2-11 are isolated from home-made yogurts manufactured in Rodopite – mountain region in Bulgaria. A new highly effective symbiotic starter culture with a high degree of proto-cooperation between strains and high technological characteristics for the production of original Bulgarian yogurt is developed from *S.thermophilus* 13a and *Lb. bulgaricus* 2-11 [Simova et al. 1999, Simova and Beshkova 2007, Angelov et al. 2002, Simova 2007].

The inoculum of monocultures and associations is prepared in the following way: after microbial and biochemical indexes control the whole cow milk is sterilized at 121° C for 15 minutes, then the milk is cooled to 43° C and is inoculated with 2% of the corresponding culture.

Batch cultivations of starter culture *S.thermophilus* 13a + *Lb. bulgaricus* 2-11 are carried out in bioreactor MBR AG Ltd. (Switzerland) with a geometric volume of 2 dm^3 and control device IMCS – 2000.

The laboratory bioreactor MBR AG Ltd. is shown in Figure 1. The bioreactor is equipped with a six-blade turbine stirrer and four repulse devices. There are two orifices on the lid: one for feeding and the other for the installation of heat exchangers, sensors for temperature, pH and dissolved oxygen. The installation includes sensors and mechanisms for monitoring and control of the main physico-chemical process variables – pH, dissolved oxygen concentration and stirrer speed.

The feed (sterilized and restored dry milk containing 12% of dry material) and inoculates are inserted in the apparatus using a peristaltic pump that is indicated with number 10 in Figure 1.



Figure 1: Laboratory bioreactor MBR AG Ltd scheme 1 - apparatus with geometric volume 2 dm³; 2 - four repulse devices; 3 – thermo-strength Pt100; 4 – heater; 5 - heat exchanger for cold water; 6 – stirrer; 7 – pH electrode; 8 – dissolved oxygen electrode; 9 – filter; 10 – peristaltic pump; 11 – flask with sterilized milk; 12 – motor; 13 - control links; 14 – control device.

Dissolved oxygen concentration could be set using the oxygen control scheme that includes a steam-sterilized electrode of 'Clark' Ingold type. The control system is calibrated in distilled water. The measurements are taken and expressed in percentage of saturation.

The partial pressure of the milk-dissolved carbon dioxide is measured by an extra outline of steamsterilized potentiometric CO_2 -electrode Ingold and CO_2 amplifier 525, Ingold (Switzerland). The system is calibrated using the method proposed by Spinnler [Spinler et al. 1987].

Prior to fermentation the milk is maintained at the temperature of 43° C for coagulation. The coagulants are kept refrigerated at 4° C.

During the fermentation, the following biochemical state variables are measured off-line: concentration of lactobacillus plus streptococci (CFU ml⁻¹), concentration of substrate lactose (g l⁻¹) and the concentration of lactic acid (g l⁻¹). Samples are taken at constant time intervals of 0.5 hour. Each experiment is carried out till the total acidity of the medium reaches 80^{0} T then the process is stopped. The number of viable cells of lactic acid bacteria is measured in CFU (cm³)⁻¹ according to the IDF Standard 117B, 1977. The lactic acid and lactose are measured by enzyme-based methods (UV test Boehringer Mannheim, GmbH Biochemica).

KINETIC'S MODELS

In general, the dynamics of a batch fermentation process is described by the material balance equations as follows:

$$\frac{dX}{d\tau} = \mu X$$

$$\frac{dP}{d\tau} = q_{P} X$$

$$\frac{dS}{d\tau} = -q_{S} X$$
(1)

Where X is the viable cells' concentration, P is the product's (lactic acid), S is the substrate's (lactose), μ , q_S and q_P are the specific growth rates of population growth, substrate consumption and metabolite production, respectively. The dependences of the specific kinetic rates on the process state variables determine the model structure [Bastin and Dochain 1990]. For the kinetics of *S.thermophilus* 13a + *L. bulgaricus* 2-11 growth, substrate consumption and product formation the following models are proposed [Biryukov 2004, Pirt 1975]:

Model 1:

$$\mu = \mu_{\max} \frac{S}{k_s + S}$$
(2a)

$$q_s = \frac{\mu}{\gamma} + m \tag{2b}$$

$$q_P = a + b\mu \tag{2c}$$

Model 2:

$$\mu = \mu_{\max} \frac{S}{k_s + S + k_i S^2}$$
(3a)

$$q_s = \frac{\mu}{Y} + m \tag{3b}$$

$$q_P = a + b\mu \tag{3c}$$

Model 3:

$$\mu = \mu_{\max} \frac{S}{k_s + S} \cdot \frac{k_p}{k_p + P}$$
(4a)

$$q_s = \frac{\mu}{Y} + m \tag{4b}$$

$$q_P = a + b\mu \tag{4c}$$

Model 4:

$$\mu = \mu_{\max} \frac{S}{k_s + S + P/k}$$
(5a)

$$q_s = \frac{\mu}{Y} + m \tag{5b}$$

$$q_P = a + b\mu \tag{5c}$$

Model 5:

$$\mu = \mu_{\max} \frac{k_p}{k_p + P} \tag{6a}$$

$$q_s = \frac{\mu}{Y} + m \tag{6b}$$

$$q_P = a + b\mu \tag{6c}$$

It can be observed that, the main difference between the five models appears in relation to the specific growth rates (a). The models for specific substrate (b) and product formation (c) rates are the same for all models. Therefore, the identification task is reduced to the identification of the most suitable relation to describe the specific growth rate, as well as the model parameters using the experimental data. The process data base is designed using generalized values from three independent experiments. The data is used for testing all models (2-6). The system of differential equations (1) is analytically solved using models (2) to (6) in a sequence. The model parameters are iteratively modified until the pre-set criteria – based on the square error between experimental and model data - are satisfied.

RESULTS AND DISCUSSION

The choice of kinetic dependences is made taking into account the expert's knowledge of the investigated process. At the beginning, the classical Monod law (2a) was tested. However, it is known from the literature that the growth kinetics of this process does not always follow this relationship [Biryukov 2004, Pirt 1975]. Therefore, in the work, models are preferred which account for growth inhibition by the substrate and/or product. The Haldane's growth kinetics (3a) was then tested as well. The results showed a reasonable dependence of cell's growth on the substrate and the product concentrations. Then the blocks of growth investigated next (4a and 5a) include the influence of substrate and product inhibition on microbial growth. It is well known that the lactic acid process is inhibited by the product concentration [Pirt 1975]. For this reason, the model of Jerusaliwski and Enganbervediev (6a) was also tested. The model describes the inhibitor effect of product concentration only. The tested models have simple structures, but they describe with good accuracy the investigated lactic acid process taking into account the experiments with different initial concentrations of milk-dissolved oxygen.

Specific lactose consumption rate (2b-6b) and product accumulation rate (2c-6c) are expressed by relations where those parameters are functions of the specific growth rate. For specific rate of product accumulation (2c-6c), the Luedeking-Piret [Pirt 1975] law is proposed to be tested. According to this law, a part of the product is continuously accumulated independent of microbial growth while the remaining part is proportional to the growth [Biryukov 2004]. Furthermore, the test of this relation is reasonable because it is specifically derived for lactic acid fermentations [Biryukov 2004, Pirt 1975]. For the lactose consumption rate (2b-6b), a relation proposed by Pirt [Pirt 1975] is recommended. This relation describes substrate consumption as a function of
specific growth rate and remains constant for microbe population viability. One part of the substrate is used for irreplaceable products of the metabolism, which have to be taken into account in the model [Biryukov 2004].

Table 1 Optimal criteria for searching of the best model to fit experimental data

DO _{int} ,	Model	Model	Model	Model	Model
[%]	1	2	3	4	5
5	16,97	16,92	9,98	10,17	10,28
10	14,76	14,76	7,96	8,22	8,16
15	11,09	11,07	7,63	7,64	7,60
20	14,98	14,88	8,42	8,64	8,57
40	12,73	12,60	7,41	7,48	7,45
90	32,30	32,34	14,41	13,33	14,31

The results concerning all the tested models are summarized in the Table 1. It can be observed that, the best results are given by Model 3. The deviations between the experimental data and the calculated values are 1.4 and 3.4 times lower then for other models. The models that include the inhibitor effect of product on bacterial growth (Models 3-5), give a better description of lactic acid production.



Figure 2: Kinetics of lactic acid process with 15% initial dissolved oxygen concentration in milk

DO _{in}	μ,	Ks	K _P	່ a ຼ	b	m
t [%]	[h⁻¹]	[g l ⁻¹]	[g l ⁻¹]	[g g ⁻¹]	[g g] 1]	[g l ⁻¹ h ⁻¹]
5	8	6,02	0,85	0,376	1,46 9	a,6.10
10	8	9,24	0,85 8	0,999	1,21 5	1,6.10 -5
15	7,60 3	8,70 5	0,78 5	1,223	1,12 1	1,2.10 -5
20	8	8,61 7	0,91	0,417	1,40 3	4,2.10 -6
40	8	5,84 5	0,71 0	1,359	1,40 3	4,2.10 -6
90	8	9,96 1	0,67 4	1,2.10 ⁻⁵	2,63 2	1,9.10 -5

Table 2 Process Model 3 parameters values

The quadratic error criteria for Model 3 shows the best values for dissolved oxygen concentrations between 5% and 20%. This result is very useful for industrial

practice. Hence, the relationships in Model 3 are chosed to be the most suitable ones to describe the process kinetics of lactic acid.

Figure 2 shows the simulation results in comparison with experimental data for the selected model. The experimental points are represented as circles and the model (1) output with kinetic dependences (4a) - (4c) represented as lines.

The multiplicative kinetic equation (4a) describes the between the specific growth rate of relation lactobacillus, substrate (lactose) concentration and the target product (lactic acid) concentration in the bioreactor. This model could be used for simulation of the process in the cases where some parameters and/or initial conditions are changed. The kinetic equation for the substrate consumption rate (4b) describes the relationship between the specific substrate consumption rate and the lactobacillus growth rate, where Y is a constant coefficient and μ is a maintainance coefficient for microorganism's viability. The kinetic equation of metabolite formation (4c) describes the relationship between the specific metabolite production rate and the specific growth rate.

The quantitative assessment of the oxygen's effect on the fermentation process can be based on the values obtained for the process parameters. Table 2 and Figure 3 indicate that the inhibitory constant K_p shows a trend of inverse proportionality to the changes of milkdissolved oxygen concentration. The growth-inhibiting effect, in the case of increasing substrate, starts at lower concentrations of the inhibiting component – lactic acid. This confirms the experimental observations i.e. that 40% of milk-dissolved oxygen is the critical concentration: at higher concentrations prolonged cultivation time deteriorates the lactic acid process to the extent of full milk coagulation.

High oxygen concentrations in milk (40%-90%) lead to an augmentation trend for the value of coefficient *b* in Eq. 4c (see Figure 4) which describes the product accumulation in the medium. This means that cell culture becomes slower in the stationary phase.



Figure 3:Effect of initial milk-dissolved oxygen concentration on inhibiting constant K_P



concentration on model coefficient b

In the case of high dissolved oxygen concentration, a decrease in viable cells titer is observed for the same fermentation time. A smaller number of cells results in slower oxygen consumption by streptococci and as a result in a delay of total process rate.

CONCLUSIONS

This work has analyzed the kinetics of yogurt starter culture production by *S.thermophilus* 13a and *Lb. bulgaricus* 2-11 focusing on the quantitative effects of different milk-dissolved oxygen concentrations on the process. When the initial concentration of milk-dissolved oxygen is within the 5% - 30% interval, negative consequences on thermophilic streptococcus and lactobacillus growth are not observed. The values of the kinetic parameters of mixed cultures are characterized by an extreme value that could be observed between 1.5 and 2 hour of fermentation.

The effect of dissolved oxygen $DO_{int} = 40\%$ is more notable on *Lb. bulgaricus* 2-11 (on starter culture respectively): its concentration decreases 3 times at the end of the specified interval. A decrease in lactobacillus concentration is mainly observed with no effect on the lactic acid process. The desired interaction between *S.thermophilus* 13a and *Lb. bulgaricus* 2-11 (3:1) can be obtained at $DO_{int} < 40\%$. In the same zone, a maximum ratio of both species becomes larger than it is technologically dsirable.

More significant is the effect of $DO_{int} = (60 - 90)\%$ on the lactic acid process and on the status of both populations. A delay of *Lb. bulgaricus* 2-11 growth is detected because of the inability of *S.thermophilus* 13a to consume that high an oxygen concentration in milk and to establish the anaerobic conditions for the growth of *Lb. bulgaricus* 2-11. This results in a delay of *Lb. bulgaricus* 2-11 growth and in a prolongation of the milk coagulation time. The increase of initial concentration of milk-dissolved oxygen from 5% to 90% leads to a proportional decrease in the specific growth rate of *S.thermophilus* 13a + *Lb. bulgaricus* 2-11 and of the rates of lactose consumption and lactic acid production.

On the basis of this investigation, two zones of DO_{int} in milk are defined whose limit is 40% of DO saturation. In each of these zones, the associated pair of lactic acid bacteria of starter culture show different behaviour.

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DESIGN AND ANALYSIS OF OIL PRODUCTION AREA – A SIMULATION APPROACH

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KEYWORDS

Continuous simulation modelling, Crude oil.

ABSTRACT

Crude oil separation processes involve many high profile control systems and equipment that costing a vast amount of investment. Any mistake in the management will cause serious aftermath. The main focuses in this paper are the design of simulation modelling of an oil production area and is used as planning, controlling and decision making tool with associated factors such as crude oil input rate, capacity of separator, quality of crude oil and number of production lines. The experiments and results analysed prove that the simulation model is merely imitating the real system and few recommendations are concluded for the optimisation of productivity.

INTRODUCTION

Crude oil surface production operations are among the most dynamic chemical processes in the engineering field due to the complexity, high profile and high safety considerations. The whole refinery systems from crude oil to final consumable products are separated into several steps together with hundreds of complicated piping and control systems. The simulated processes in this paper include 2-phase and 3-phase separation to filter out the water and gas from crude oil. Due to the dynamical process behaviours and great competition in same industries, manufacturers always find it difficult to achieve high performance and thorough planning using traditional designs and analytical methods. The risk and cost are too great and too high for implementations which are not fully tested and analysed for its effectiveness. Mismatches and factors that come out unexpectedly are really worrying most of the operation planners as a result of failure to the systems and enormous losses both timely and financially.

The purpose of this paper is set to use simulation tools to help in design and analysis of oil production field. The model was initially designed and simulated to match the current real system, which was later used as a planning tool to help practitioner in decision making process. The behaviours of the separation systems are to be described; the processes and theories constructed and predictions made by analysing the results from the simulation. Factors affecting the separation outcomes could be added into the model for better integrity and more precise experimentations. The modelling and simulation enables engineers to visually observe every single step and effects caused by different factors introduced into the systems. Planners are able to evaluate physical layout, selection of facilities and equipments and operational procedure changes. Processes could be altered and tested repetitively at minimum cost and time without taking on the risk of failure.

The simulation model built is to be used in examining the effect of various parameters on the performance measurements for planning and control of production systems. Integrated user friendly interface are developed for variable set up enabling different experiments to be carried out easily.

LITERATURE REVIEW

While the level of oil reserved decreased over the world,

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) higher optimisation in production systems and facilities are important to ensure the profitability. This paper focuses on the early stage of the separation process which included the vertical and horizontal separators. Air, water and oil were all separated from crude oil before being delivered for further stage of treatment.

There are various researches and works reported in the past to search for more effective optimisation approaches in oil production industries. Mathematical programming is one of the most widely implemented methods for modelling with the objective to maximise the profitability. Linear programming is a popular example in mathematical programming introduced for planning of maintenance shut-down and stock control. The theories of linear programming was developed further by Ballintijn (1993) and presented by Giliberti et. al (1995) for optimisation of the dynamic simulation at a giant oil field.

Shah (1996) used mathematical programming techniques for crude oil scheduling which is applicable to hybrid approach. Fichter (2000) showed that application of Genetic Algorithms in oil and gas portfolio optimisation was excellent at handling accurate and complex, non linear business model. Hansen (2001) discussed the distribution of the multi-phase fluid flow in a horizontal gravity separator. Computational Fluid Dynamics (CFD) could provide valuable insight, and the fluid flow behaviour in the liquid volume flow zone inside the separator was analysed and simulation was performed. Yu et. al. (2004) introduced an approach for solving the problem of bending optimisation based on history data and the effectiveness of proposed model were shown by using real data of oil field which, however, been criticised the design procedure of conventional oil-water separation was to be improved.

Rincon et. al. (2005) proposed a set of criteria for evaluating discrete-event simulation software capable of simulating continuous operations with a quality specifications model developed and demonstrated at a consultancy in Venezuelan oil industry. Apart from the technologies, strategy was another important method of optimising the productivity of oil. Tavares et. al. (2006) assessed different strategies for the expansion of Brazil oil refinery segments, using criteria that range from energy security (reducing imports and vulnerability for key products) through to minimising the profitability of this sector (boosting the output of higher value oil products) and adding value to Brazil's oil production (reducing exports of heavy acid oil).

Although most of the previous research that have been carried out were mostly focussing on optimising the production using linear programming, statistical analysis, mathematical solutions and critical path analysis, simulation was one of the methods mostly chosen after statistical analysis as an operation research tool (The British Petroleum, 1977).

RESEARCH METHODOLOGY

What are modelling and computer simulation? Modelling is a way to represent a group of objects ideas and behaviours of different systems and processes in the form of either physically or logically. Maki and Thompson (2006) differentiated the types of model into physical models, theoretical models, logical models, computational models, simulation models and mathematical models.

Mathematical models can be analysed through mathematics, theories, differential equations, partial-differentiation equations, diagrams and tables. It is also a set of process with approximation and assumptions attempts to match observation with logical or symbolic statements. Mathematical models are mostly simplified and idealised to identify the most important parts to be modelled especially in the prediction of the outcomes which is called 'real model'. Although it can provide the accuracy and precision of predictions, decisions and explanations, the model can be developed into more complex and difficult design when dealing with complicated systems.

A heuristic model can be used to seek immediate solutions in short time despite the feasibility or

optimality. Nevertheless, there is a concern that it is likely to be erroneous and is unable to guarantee the accuracy to problems being solved.

Simulation modelling or computer simulation is chosen for this research work due to its powerful ability in dealing with either simple or complex systems which are more preferable. Computer simulation is a process of designing a digitalised model representing a real or a proposed system for the experimentation purpose and understanding of the system's actual behaviours with given factors and scenarios.

Simulation in the oil and gas industry allows managers and engineers obtaining a system wide view of the effect from local changes to the production area. Computer simulation is beneficial in cost saving, time saving, comparison of different scenarios especially in the impossibility of real system construction, wide areas of implementation, answering 'what-if' questions, the competencies and ease of use for supporting decision making. Other advantages are (i) advances in software technology where programming language improves the software power for rapid and valid decision making, (ii) provides training to operators without affecting the real operations, (iii) a better insight and understanding in visualisation of operations systems gained through animation in simulation model advancements.



Figure 1: Framework in simulation study

Time and variability are the two most important aspects when designing a simulation model. Three main categories of simulation model classified by Kelton et. al (2007) are static versus dynamic, discrete versus continuous, and deterministic versus stochastic. This project has both discrete but mostly regarded to continuous systems. In continuous environment, the system could work around the clock without break except for maintenance. Examples of such system are the utilities companies, petrochemical factories, oil industries, etc. Figure 1 shows the framework of the general simulation process.

There are various simulation software tools in the market which are targeting at different industries. ARENA simulation tool from Rockwell Software was chosen as the simulation tool in this research project for advantages in higher performance, moderate modelling duration, developed skills in the software applications and ease of use of the software tool.

CRUDE OIL SEPARATION UNITS

A perfect model is preferable at all time by the modeller, nonetheless, this is not always possible due to the difficulties in obtaining full data required for real systems design.

A conceptual model is necessary to combining all the objectives of simulation, inputs variables, outputs performance and assumptions made to simplify the model. Figure 2 explains the process flow of the crude oil separation from early stage until the end of the process for delivery to the port. The amount of gas, water and oil from each stage to another differs according to the pressure of separators and contents of the hydrocarbon in crude oil delivered from wells.

Data collection and assumptions

The proposed model and the data collected are based on a real oil production area in one of the developing countries. Data collected were analysed and further assumptions and calculations were made in order to find out the rest of data required for modelling. Therefore, the more data gathered, the more accurate the simulation model could be designed.



Figure 2: Process Flow Chart of Crude Oil Separation

Model constructions

Due to the complexity and great size of the model, few selected parts of the model are explained and discussed. Four different entities were created at time zero and were used to trigger the crude oil separation process in Arena software. Each of these entities was assigned with their own attributes for the computer to understand their characteristics and identity. The 'seize' module seized the manifold output regulators and the input regulators which is particularly available for the assigned entities.

The flow rate of the transfer between manifold and Stage 1 separator was adjusted by the 'regulate' module. Different pre-recorded values of input flow rate were available for users to choose and these would lead to different utilisation of the separator as well. The model would automatically show the latest utilisation of separator according to the number of crude oil production line activated. By referring to Figure (3-a and 3-b), the entity will go through a series of process to check if the level of separators was in the allowed limit. A sensor was used to represent the level valve in real system to detect the level of crude oil in the manifold. The entity was entered into the line for lowering the regulator rates, or vice versa, otherwise it was disposed for not meeting the requirements of design. The entity that met the requirements would then circulate in the loop until the end of the process.



Figure 3-a: Crude Oil Separation at Stage 1



Figure 3-b: Crude Oil Separation at Stage 1

Another entity was created in next stage to activate the flow from stage 1 to stage 2 separators. Same procedure

was applied to the process from stage 2 to stage 3, stage 3 to stage 4 and stage 4 to stage 5 until the end of the production line by creating different entities. Extra entities were duplicated to activate the flow of gas and water at same stage of process when the entities entered the systems. At the end of the production line, the entities were able to choose the storage tank for storage depending on the availability of space.



Figure 4: Overall modelling view of the simulated environment

Verification and validation

This crude oil separation model was verified by checking on the model codes, visually checking and inspecting of output reports. Any changes made were all recorded and could be referred back by the modellers and users. Visually checking method was carried out of ensuring the event and entity occurred and moved at the right sequence. A step forward button was used in checking the event happened at every step. The speed could be reduced to allow more time for entity movement observation. Animation was useful in the visual checks apart from stepping through the logic modules. Both visual checking by analysing the animation as shown in Figure 4 and tracing of the entity over time were applied together for the best model verification results.

A simpler version of the model was built with the whole process and results were compared to real systems for validation process. The simple model was then expanded to more complicated design and continuously tested, verified and validated to avoid any mistiness searching for errors when the model grew more complex.

EXPERIMENTATIONS, RESULTS ANALYSIS AND DISCUSSIONS

Factorial designs are the common experimental design that most people used such as 2^k or 3^k . However, the experiments carried out in this simulation model contain more than three levels. Mixed factorial designs are more appropriate. Two types of experiments are carried out. First experiment is based on the interaction of crude oil arrival input rates, number of production lines and quality of crude oil. Second type of experiment is based on interaction of crude oil arrival rates, number of production lines and capacity of separator. Both experiments are based on $2^4 \times 7$ which is 112 runs and $2^4 \times 3$ with 48 runs. An extra experiments are carried out that examine the relationship between crude oil input rates and separator capacity.

Total of 177 runs were completed and results were displayed in figure 5, 6, 7 and 8. Four different crude oil input regulator rates were used in this model and were increased from 5433.62bbl/min to 21734.47bbl/min throughout the four sets of experiments. From the results in figure 5, the oil output rate was decreased linearly with lower quality oil even when the number of activated lines was increased. It is obvious that the more production lines activated, the more oil output produced at the end of production. However, the declines are caused by the increment of the water in the crude oil.

Figure 6 displays the relationship between the input and output rates, as expected the output rate increases as the input rate increases, however, we could not experiment with higher input rate more than +125% as the utilisation was found to be almost 100%.

Figure 7 compares the effect of different crude oil input rates on the utilisation of the separators. The input rates were reduced or increased from their original figures gradually in the range of -75% to +75% to optimise the separation process and avoid any over flow in the system. As can be seen in figure 7, the utilisation was increased gradually at the same time when the input rates were increased. The minimum utilisation was found at 50% while the maximum was almost 99%.



Figure 5: Oil output versus quality of crude oil



Figure 7: Separator utilisation versus input rate

In figure 8, the crude oil input rates are kept at original value. This is to compare and to show the importance of balance between input rate and capacity of separator. Any separator sized less than original capacity would not be able to cope with the original input rate of 21734.47 barrel/min, which means the separator is over utilised. In fact, any separator sized bigger than original capacity will have no effect on the amount of oil output which means it is under utilised. At points -35 percents or less, there were zero oil output. This happened since the model was designed to dispose the entity created in simulation if there is an enormous amount of crude oil input entered the system which might cause dangerous situation.

Through the analysis of the results and graphs, it is obviously notified that the crude oil input rate is the main criteria to decide the amount of oil output. However, co-factors which affect the output are the quality of crude oil, capacity of separator and number of production lines. This model shows that it is able to simulate the system, process and give a reliable outcome based on the criteria set. Some user interface dialogue



Figure 6: Oil output versus input rate



Figure 8: Oil output versus separator's capacity

boxes are designed to enable users to modify the value of the factors.

CONCLUSIONS, RECOMMENDATIONS AND FURTHER WORKS

Cost reduction is a major benefit for using simulation in spite of having real implementation for testing out the plans or design in the crude oil separation system without building up or taking out any facilities. The animation designed based on the modelled system provides the users with a clear overview on what is happening throughout the process for better understanding and confident in planning and decision making without taking risk of unworkable solutions.

Although this proposed simulation model has its beauties and advantages, the accuracies are all depend on the skills of the modeller, time period and detailed data provided/collected and power of the software tool to handle such design. Due to lack of complete data, this model was slightly simplified and assumptions were made to meet the reliability as representation of the real system. Validation of the model was hindered due to lack of data and unavailability of similar models in the literature using simulation tool. Overall, the testing results and experiments were very closely equal to actual results and this model could imitate the real production system only based on the four factors.

All the four factors taken into account of the design are all inter-related to each other. Crude oil input rate is considered as the main factor to decide the amount of oil output. The utilisation of the separators indicated the importance of balance between crude oil input rate and the load the separator could take. Over utilisation would cause failure to the whole system while under-utilisation meant the lower profitability.

Recommendations

The production planning is important for understanding what is the average production needed over years and if the supply of crude oil is enough for the demands. It is recommended that crude oil quality should be pre-investigated to ensure lower water content. Capacity of separator should be finely justified with its utilisation with commonly at 60 percents to allow the reduction and increase of productivity when necessary. Make to order is more likely to be cost-effective way to minimise extra production and storage cost. However, minimum stock should be kept for emergency like strike or problems in production system. Productivity can be increased by increasing the crude oil input rate and more production lines created only with good counterpoise between cost and profit.

Further work

This model can be designed with some differentiation equations for better estimation of the output within a range of input rates instead of specific values set in advance. More advanced VBA code can help to enhance the flexibility of the system in handling the changing of the input rates with coordination with the differentiation equations. Framework and model integration with other application software like Microsoft Excel and Access could be explored more in order to provide more function and ease of use to the user through programming. More factors affecting the crude oil separation could be included for handling various complicated scenarios.

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Simulation of Intelligent Systems

Methodology of Parallel Programming using Compositions of Parallel Objects or CPANS for the solution of NP-Complete problems

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KEYWORDS

Parallel Objects, Structured Parallel Programming, HighPerformanceComputing,ObjectOrientedProgramming, Concurrent Programming, CPANs.

ABSTRACT

Within an environment of Parallel Objects, an approach of Structured Parallel Programming and the paradigm of the Orientation to Objects, shows a programming method based on High Level Parallel Compositions or HLPCs (CPANs in Spanish) by means of classes. The synchronous, asynchronous communication ways and asynchronous future of the pattern of Parallel Objects (Rossainz and Capel 2005-2), the predefined patterns of communication/interaction of the structured approach, the encapsulation and the abstraction of the Orientation to Objects, to provide reusability to this patterns, together with a set of predefined restrictions of synchronization among processes (maxpar, mutex, sync) are used. The implementation of the commonly used communication patterns is explained, by means of the application of the method, which conform a library of susceptible classes of being used in applications within the environment of programming of the C++ and of the standard POSIX of programming with threads such as the solution to the Travelling Salesman Problem (TSP) by means of the parallel Branch & Bound technique like a CPAN.

INTRODUCTION

As it is known, exist infinity of applications that using machines with a single processor tries to obtain the maximum performance from a system when solving a problem; however, when such a system can not provide the performance that is required (Capel and Troya 1994), a possible solution it consists on opting for applications, architectures and structures of parallel or concurrent processing. The parallel processing is therefore, an alternative to the sequential processing when the limit of performance of a system is reached. In the sequential computation a processor only carries out at the same time an operation, on the contrary of what happens in the calculation parallel, where several processors they can cooperate to solve a given problem, which reduces the time of calculation since several operations can be carried out simultaneously. From the practical point of view, today in day is enough justified carrying out compatible investigations within the area of the parallel processing and areas related (Concurrence, Distributed Systems, Systems of Real Time, etc.), since the recent advance in massively parallel systems, communications of great band width, quick processors for the treatment of signs, etc., they allow this way it. Important part of those investigations are the parallel algorithms, methodologies and models of parallel programming that at the moment are developing. The parallel processing includes many topics that include to the architectures, algorithms, languages of programming parallel and different methods of performance analysis, to mention some of the most excellent.

The present investigation centers its attention in the Methods of Structured Parallel Programming, proposing a new implementation with C++ and the library of threads POSIX of the programming method based on the pattern of the High Level Parallel Compositions or CPANs (Corradi 1995; Danelutto), the which it is based on the paradigm of Orientation to Objects to solve problems parallelizable using a class of concurrent active objects. In this work supply a library of classes provides that the programmer the communication/interaction patterns more commonly used in the parallel programming, in particular, the pattern of the pipeline, the pattern denominated farm and the pattern tree of the technique Divide and Conquer of design of algorithms, well-known as it.

MOTIVATION

At the moment the construction of concurrent and parallel systems has less conditioners every time, since the existence of systems parallel computation of high performance, or HPC (High Performance Computing), more and more affordable, has made possible obtaining a great efficiency in the processing of data without the cost is shot; even this way, open problems that motivate the investigation in this area still exist; in particular, interest us those that have to do with the parallel applications that use communication patterns predetermined among their component software. At the moment are identified as important open problems, at least, the following ones:

The lack of acceptance of environments of parallel programming structured to develop applications: the

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) structured parallelism is a type of parallel programming based on the use of communication/interaction patterns (pipelines, farms, trees, etc.) predefined among the processes of user's application. The patterns also encapsulate the parallel parts of this application, of such form that the user only programs the sequential code of this one. Many proposals of environments exist for the development of applications and structured parallel programs, but until the moment, they are only used by a very limited circle of expert programmers. At the moment, in HPC, a great interest exists in the investigation of environments as those previously mentioned ones.

The necessity to have patterns or high level parallel compositions: a high level parallel composition or CPAN, as well as is denominated in (Corradi 1995), it must be been able to define and to use within an infrastructure (language environment or of programming) oriented to objects. The components of a parallel application not interaction in an arbitrary way, but regular basic patterns follow (Hartley 1998). An environment of parallel programming must offer its users a set of components that implement the patterns or CPANs more used in algorithms and parallel and distributed applications, such as trees, farms, pipes, etc. The user, in turn, must can to compose and to nest CPANs to develop programs and applications. The user must be limited to a set of predefined CPANs, but rather, by means of the use of the inheritance mechanism, he must can to adapt them to his The development environment must necessities. contemplate, therefore, the concept of class of parallel objects. Interest exists in exploring the investigation line related with the definition of complete sets of patterns, as well as in its semantic definition, for concrete classes of parallel applications.

Determination of a complete set of patterns as well as of their semantics: in this point, the scientific community doesn't seem to accept in a completely satisfactory way and with the enough generality none of the solutions that have been obtained to solve this problem today. It doesn't seem, therefore, easy the one that can be found a set the sufficiently useful and general thing, for example a library of patterns or set of constructos of a programming language, to be used in the development, in a structured way, of a parallel application not specific.

Adoption of a approach oriented to objects: Integrating a set of classes within an infrastructure oriented to objects is a possible solution to the problem described in the previous point, since would allow adding new patterns to an incomplete initial set by means of the subclasses definition. Therefore, one of the lines of followed investigation has been finding representations of parallel patterns as classes, starting from which instance parallel objects is been able to (CPANs) that are, in turn, executed as consequence from an external petition of service to this objects and coming from user's application. For example, the derived pattern of the execution for stages of the processes would come defined by pattern's denominated pipeline class; the number of stages and the sequential code of each specific stage would not be established until the creation of a parallel object of this class; the data to process and the results would be obtained of user's application; the internal storage in the stages could adapt in a subclass that inherits of pipeline. Several advantages are obtained when following a approach oriented to objects (Corradi and Leonardi 1991), regarding a approach only based on skeletons algorithmic and programs model (Hartley 1998), it is necessary to point out, for example, the following improvements:

Uniformity: All the entities within the programming environment are objects.

Genericity: The capacity to generate references dynamically, within an environment of software development oriented to objects, makes possible the creation of generic patterns, by means of the definition of its components as generic references to objects. Reusability: The inheritance mechanism simplifies the definition of specialized parallel patterns. The inheritance applied to the behavior of a concurrent object helps in the specification of the parallel behavior of a pattern.

EXPOSITION OF THE PROBLEM

From the work carried out to obtain the investigating sufficiency. redefining and modernizing the investigation, the problem to solve is defining a Parallel Programming Method based on High Level Parallel Compositions (CPANS) (Corradi 1995). For it the following properties have considered as indispensable requirements that should be kept in mind for the good development of this investigation. It is required, in principle, a environment of Programming Oriented to Objects that it provides: Capacity of invocation of methods of the objects that contemplates the asynchronous communication ways and asynchronous future. The asynchronous way doesn't force to wait the client's result that invokes a method of an object. The asynchronous future communication way makes the client to wait only when needs the result in a future instant of her execution. Both communication ways allow a client to continue being executed concurrently with the execution of the method (parallelism interobjects).

The objects must can to have internal parallelism. A mechanism of threads it must allow to an object to serve several invocations of their methods concurrently (parallelism intra-objects).

Availability of synchronization mechanisms when parallel petitions of service take place. It is necessary so that the objects can negotiate several execution flows concurrently and, at the same time, to guarantee the consistency of their data.

Availability of flexible mechanisms of control of types. The capacity must be had of associating types dynamically to the parameters of the methods of the objects. It is needed that the system can negotiate types of generic data, since the CPANs only defines the parallel part of an interaction pattern, therefore, they must can to adapt to the different classes of possible components of the pattern.

Transparency of distribution of parallel applications. It must provide the transport of the applications from a system centralized to a distributed system without the user's code is affected. The classes must maintain their properties, independently of the environment of execution of the objects of the applications.

Performance. This is always the most important parameter to consider when one makes a new proposal of development environment for parallel applications. A approach based on patterns as classes and parallel objects must solve the denominated problem PPP (Programmability, Portability, Performance) so that it is considered an excellent approach to the search of solutions to the outlined problems.

The environment of programming oriented to Objects that it has been considered as suitable to cover the 6 previously mentioned properties is the programming language C++, together with the use of the standard POSIX Thread.

SCIENTIFIC OBJETIVES OF INTEREST

The development of a programming method is based on High Level Parallel Compositions or CPANs that implement a library of classes of utility in the Programming Concurrent/Parallel Oriented to Objects (Rossainz 2005). The method must provide the programmer the commonly used parallel patterns of communication, in such a way that this can exploit the generalization mechanisms for inheritance and parametrization to define new patterns according to the pattern of the CPAN.

HIGH LEVEL PARALLEL COMPOSITIONS OR CPANS

Some of the problems of the environments of parallel programming it is that of their acceptance for the users, which depends that they can offer complete expressions of the behavior of the parallel programs that are built with this environments (Corradi 1995). At the moment in the systems oriented to objects, the programming environments based on parallel objects are only known by the scientific community dedicated to the study of the Concurrence.

A first approach that tries to attack this problem it is to try to make the user to develop his programs according to a style of sequential programming and, helped of a system or specific environment, this can produce his parallel tally. However, intrinsic implementation difficulties exist to the definition of the formal semantics of the programming languages that impede the automatic parallelization without the user's participation, for what the problem of generating parallelism in an automatic way for a general application continues being open. A promising approach alternative that is the one that is adopted in the present investigation to reach the outlined objectives, is the denominated structured parallelism. In general the parallel applications follow predetermined patterns of execution. These communication patterns are rarely arbitrary and not structured in their logic (Brinch Hansen 1993). The High Level Parallel Compositions or CPANs are patterns parallel defined and logically structured that, once identified in terms of their components and of their communication, they can be taken to the practice and to be available as abstractions of high level in the user's applications within an environment or programming environment, in this case the one of the orientation to objects. The structures of interconnection of more common processors as the pipelines, the farms and the trees can be built using CPANs, within the environment of work of the Parallel Objects that is the one used to detail the structure of the implementation of a CPAN.

Definition of the pattern CPAN

The basic idea is the one of implementing any type of parallel patterns of communication between the processes of an application or distributed/parallel algorithm as classes, following the paradigm from the Orientation to Objects. Starting from this classes, an object can be instanced and the execution of a method of the object in question you can carry out through a petition of service. A CPAN comes from the composition of a set of objects of three types (Rossainz and Capel 2005-2):

An object manager (Figure.1) that it represents the CPAN in itself. The manager controls the references of a set of objects (an object Collector and several objects Stage) that represent the components of the CPAN and whose execution is carried out in parallel and it should be coordinated by the own manager.



Figures 1: Component MANAGER of model CPAN

The objects Stage (Figure.2) that are objects of specific purpose, in an interface type client-server that settles down between the manager and the objects slaves (external entities that contain the sequential algorithm that constitutes the solution of a given problem).



Figures 2: Component Stage of model CPAN and its associated slave object.

And an object Collector (Figure.3) that it is an object that storing in parallel the results that he receives of the objects stage that has connected.



Figures 3: Component Collector of model CPAN

Composition of the CPAN.

In summary, a CPAN is composed of an object manager that it represents the CPAN in itself, some objects stage and an object of the class Collector, for each petition that should be treated within the CPAN. Also, for each stage, an object slave will be taken charge of the implementation of the necessary functionalities to solve the sequential version of the problem that you pretend to solve (Figure.4).



Figures 4: Internal structure of a CPAN. Composition of its components

The CPAN seen as composition of parallel objects.

The objects manager, collector and stages are included within the definition of Parallel Object (PO) (Corradi 1995). The Parallel Objects are active objects that have execution capacity in themselves. An object PO has a similar structure to that of an object in Smalltalk, but it also includes a politics of scheduling that specifies the form of synchronizing an or more operations of a class in parallel. The synchronization policies are expressed in terms of restrictions; for example, the mutual exclusion in processes readers/writers or the maximum parallelism in processes writers.

Types of communication in the parallel objects.

The parallel objects define 3 communication ways

- 1. **The synchronous way** stops the client's activity until the object active server gives him the answer.
- 2. The asynchronous way doesn't force the wait in the client's activity; the client simply sends the petition to the object active server and her execution continues.
- 3. The asynchronous future way makes only wait the client's activity when, within its code, the result of the method is needed to evaluate an expression.

The Synchronization restrictions MaxPar, Mutex y Sync.

It is necessary having synchronization mechanisms, when parallel petitions of service take place in a CPAN, so that the objects that conform it can negotiate several execution flows concurrently and, at the same time, guarantee the consistency in the data that are processing. Within any CPAN the restrictions MAXPAR (The maximum), MUTEX (mutual exclusion among processes that want to consent to a shared object) and SYNC (synchronization of the type producer/consumer) can be used for the correct programming of their methods.

DESIGN AND CONSTRUCTION OF THE CPANS FARM, PIPE Y TREEDV

The parallel patterns worked in the present investigation have been the pipeline, the farm and the treeDV to be a significant set of reusable patterns in multiple applications and algorithms.

- 1. **The pipeline**, this compound for a set of interconnected states one after another. The information follows a flow from a state to another.
- 2. **The farm**, is composed of a set of worker processes and a controller. The workers are executed in parallel until reaching a common objective. The controller is the one in charge of distributing the work and of controlling the progress of the global calculation.
- 3. In the treeDV, the information flows from the root toward the leaves or vice versa. The nodes that are in the same level in the tree are executed in parallel making use of the denominated technique of design of algorithms it Divide and Conquer for the solution of the problem.

These parallel patterns conform the library of classes proposed within the pattern of the CPAN.

The Cpan PipeLine

It is presented the technique of the parallel processing of the pipeline as a High Level Parallel Composition or CPAN, applicable to a wide range of problems that you/they are partially sequential in their nature. The CPAN Pipe guarantees the parallelization of sequential code using the patron PipeLine (see figure 5).



Figures 5: The CPAN of a Pipeline

The CPAN Farm

It is shown the technique of the parallel processing of the FARM as a High Level Parallel Composition or CPAN. The representation of parallel pattern FARM as a CPAN is show in Figure. 6.



Figures 6: The Cpan of a Farm

The Cpan TreeDV

Finally, the programming technique is presented it Divide and Conquer as a CPAN, applicable to a wide range of problems that can be parallelizable within this scheme (see Figure. 7).



Figures 7: The Cpan of a TreeDV

RESULTS OBTAINED

Some CPANs adapt better to the communication structure of a given algorithm than others, therefore yielding different speedups of the whole parallel application.

We carried out a Speedup analysis of the Farm, Pipe and TreeDV CPANs for several algorithms in an Origin 2000 Silicon Graphics Parallel System (with 64 processors) located at the European Center for Parallelism in Barcelona (Spain) this analysis is discussed below.

Assuming that we want to sort an array of data, some CPANs will adapt better to communication structure of a Quicksort algorithm than others. These different parallel implementations of the same sequential algorithm will therefore yield different speedups.

This analysis of speedup of the CPANs appears in Figures 8, 9 and 10. In all cases the implementation and test of the CPANs Farm, Pipe and TreeDV 50000 integer numbers were randomly generated to load each CPAN.



Figures 8: Scalability of the Speedup found for the CpanFarm in 2, 4, 8, 16 and 32 processors



Figures 9: Scalability of the Speedup found for the CpanPipe in 2, 4, 8, 16 and 32 processors



Figures 10: Scalability of the Speedup found for the CpanTreeDV in 2, 4, 8, 16 and 32 processors

PARALLELIZATION OF BRANCH & BOUND TECHNIQUE

Branch-and-bound (BB) makes a partition of the solution space of a given optimization problem. The entire space is represented by the corresponding BB *expansion tree*, whose root is associated to the initially unsolved problem. The children nodes at each node represent the subspaces obtained by *branching*, i.e. subdividing, the solution space represented by the parent node. The leaves of the BB tree represent nodes that cannot be subdivided any further, thus providing a final value of the cost function associated to a possible solution of the problem. Three stages are performed during the execution of a program based on a BB algorithm,

- 1. *Selection:* A node belonging to the set of live nodes, i.e. those not pruned yet, is extracted. Node selection depends on the strategy search on the live node list, which was previously decided for its use in the algorithm.
- 2. *Branch:* the node selected in the previous step is subdivided in its children nodes by following a ramification scheme to form the expansion tree. Each child receives from its father node enough information to enable it to search a suboptimal solution.
- 3. **Bound:** Some of the nodes created in the previous stage are deleted, i.e. those whose partial cost, which is given by the cost function associated to this BB algorithm instance, is greater than the best minimum bound calculated up to that point.

The ramification is generally separated from the bounding of nodes on the expansion tree in parallel BB implementations. Each object node of the expansion tree must contain all the necessary information to be an active object.

The ramification and bounding are implemented using the CPAN Farm of the proposed library, so that the ramification and the distribution of work to the application processes are carried out by using *the Farm communication scheme*. The expansion tree, for a given instance of the BB algorithm, is obtained by iteratively subdividing the stage objects according to the farm pattern until a stage representing a leaf-node of the expansion tree is found, see Figure 11. On the other hand, the pruning is implicitly carried out within another *farm* construction by using a *totally connected scheme* between all the processes. The manager can therefore communicate a sub-optimal bound found by a process to the rest of branching processes to avoid unnecessary ramifications of sub-problems, i.e., those that do not lead to improving the best upper bound obtained up to that moment.



Figures 11: The Cpan Branch & Bound

Speedup of CpanBB in the solution of Travelling Salesman Problem (TSP)

With the model of the Cpan Branch & Bound we have been able to offer an optimal solution of a Travelling Salesman Problem (TSP) NP-Complete problem (GoodMan and Hedetniemi, 1977), with 50 cities and by using the first best search strategy driven by a least cost function associated to each live node (Capel and Palma, 1992). The results obtained yielded a deviation ranging from 2% (2 processors) to 16% (32 processors) with respect to the optimal ones, as predicted by the Amdalh law for this parallelized algorithm. See Table 1 and Figure 12.

					CPU1	CPU
	Seq	CPU2	CPU4	CPU8	6	32
Run	35.42	21.88	14.21	11.34	10.27	9.10
time	Seg.	Seg.	Seg.	Seg.	Seg.	Seg.
Time Usuary	25.80 Seg.	22.14 Seg.	20.16 Seg.	18.16 Seg.	21.67 Seg.	21.1 4 Seg.
Time System	1.30 Seg.	1.11 Seg.	1.01 Seg.	1.03 Seg.	1.02 Seg.	1.04 Seg.
Time CPU	27.10 Seg.	23.25 Seg.	21.17 Seg.	19.19 Seg.	22.69 Seg.	22.1 8 Seg.
Cycles	2669 4871 9	69877 161	69073 500	67663 433	66942 422	6599 2570
Instruct ions	2021 0611 2	73380 571	73219 450	72932 731	72454 022	7223 5919
CPI	1.321	0.952	0.943	0.928	0.924	0.91 4
Speed Up	1.00	1.62	2.49	3.12	3.45	3.89
Amdalh	1.00	1.68	2.55	3.43	4.16	4.64

Table 1: Statistics of Speedup the CpanBB



Figures 12: Speedup of parallel CpanBB_tsp with N=50 cities in 2, 4, 8, 16 and 32 processors

This analysis of Speedup of the CPANS B&B was carried out also in the Origin 2000 Silicon Graphics Parallel System; see (Rossainz and Capel, 2005) for details.

CONCLUSIONS

An programming method has been presented, which is based on the High Level Parallel Compositions of Corradi , but updated and adapted to be used with C++ programming language and POSIX standard for thread programming. Several patterns of communication/interaction between processes have been implemented as generic, reusable library of CPANs, which can even be used by inexperienced parallel application programmers to obtain efficient code by only programming the sequential parts of their applications.

The CPANs Pipe, Farm and TreeDV conform a first version of a library of classes intended to be applied to the solution of several complex problems, as the parallelization of the B&B technique to offer an optimal solution of the TSP NP-Complete problem.

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FLOW SHOP SCHEDULING USING CLUSTERED DIFFERENTIAL EVOLUTION

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KEYWORDS

Differential evolution, flowshop scheduling, clustering

ABSTRACT

A generic approach of population dynamics and clustering for permutative problems is presented in this paper. Diversity indicators are created from solution ordering and its mapping is shown as an advantage for population control in metaheuristics. Differential Evolution Algorithm is embedded with a population based on this approach and vetted with the Flow shop scheduling problem. Extensive experimentation is conducted on benchmark problems in this area with good results.

INTRODUCTION

Metaheuristics are algorithms, which are used for the optimization of complex systems. The vital attribute for these heuristics is that they have to operate without apriori information of the system.

Metaheuristics operate on two ideological frameworks, firstly that a group of solutions provide a better platform to find optimal solution, and secondly that certain guiding concept leads the solutions towards the optimal solution, or nearby regions.

A number of different transformation concepts have evolved within the scope of Metaheuristics (Dreo et al., 2006). Genetic Algorithms, Differential Evolution, Particle Swarm Optimization and Self Organising Migrating Algorithm are some of the most potent heuristics available. Most of these algorithms have mimicked naturally occurring phenomena.

The principle concept of the population is to provide a pool of solutions from which the optimal solution evolves from, however during the subsequent transformation, the solutions cluster together in nearby neighbourhoods. This leads to the loss of diversity of the solutions, and later generations are usually mutating within a cloned gene pool. This phenomenon is generally termed as stagnation and the two most current correcting tools are local search within the hierarchical population and forfeiting of some better-placed solutions in lieu of worst ones (Onwubolu (2002)). Godfrey Onwubolu, Knowledge Management & Mining, Richmond Hill, Canada. Email: onwubolu_g@dsgm.ca

Stagnation is a major concern for evolutionary heuristics, since evolution is principally based on diversity of the existing population. The preconception that extended generations of a heuristic will lead to better solutions is nonviable for a stagnated population.

This paper is devoted to the concept of the population and its controlling dynamics. It is shown through experiment that population control is an effective tool in sustaining the diversity of the population, which in turn leads to more viable regions of search space for exploration.

1 POPULATION DYNAMICS

One of the most challenging optimization problems is *permutative based* combinatorial optimization. This class of problem, harbours some of the most famous optimization problems like travelling salesman (TSP) and vehicle routing problem (VRP).

What makes a permutative problem complex is that the solution representation is very concise, since it must have a discrete number of values, and each occupied variable in the solution is unique. Given a problem of size n, a representation can be described as $x = \{x_1, x_2, x_3, ..., x_n\}$, where each value x_1 in the solution is unique and the entire set of solutions is an integer representation from $\{1, n\}$.

From an optimization point of view, this represents a number of problems. Firstly, the search space is discrete and a number of validations inevitably have to be conducted in order to have a viable solution. Secondly, the search space is very large, to the scale of n!. Consequently, these problems are generally termed NP or NP Hard (Hochbam (1997)).

The usual approach is to explore the search space in the neighbourhood of good solutions in order to find better solutions. This unfortunately has the effect of converging the population, which then leads to stagnation. The usual term is *local optima convergence/stagnation*.

This research looks at the *diversity* of the population in order to aid the application of metaheuristics. A permutative solution and its representation present some advantages to this effect. The usual measure of a solution is its fitness, in respect to the problem being solved. In a permutative solution, the distinct ordering of values gives

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) the opportunity to have other measures of diversity.

The following sections describe the approach developed within this scope of research. The first part discusses the need for having distinct initial population. The second part describes some fields of measure of diversity followed by the approach of clustering of the solutions. Differential Evolution Algorithm is then presented to which the clustered population has been applied. The subsequent sections describe the extensive experimentation conducted on Quadratic Assignment problems and analysis of the dynamic nature of clustering populations.

1.1 Initial Population

The basic concept is to have a "clustured" population. This is an ideal position from which to guage the effectiveness of the heuristic. Also, this provides a better initial point for scheduling problems. An ideal explanation is the TSP, where adjacent cities usually provide minimal travel distance.

The initial population, P, for this heuristic is partially stochastic and partly deterministic. The population is divided into n sub-populations, SPs, n/2 randomly generated (SP_{rand}) and the rest structurally generated (SP_{struct}).

The formulation for SP_{rand} is fairly simple. A random permutative string is generated for each solution till a specified number given as P_{size} .

The structured population SP_{struct} is somewhat more complex. It is made of two parts. In the first part an initial solution is generated with ascending values given as $x_{ascending} = \{1, 2, 3, .., n\}$, where *n* is the size of the problem. In order to obtain a structured solution, the first solution is segmented and recombined in different orders to produce different combinations. The first segmentation occurs at n/2 and the two halvess are swapped to produce the second solution. The second fragmentation occurs by the factor 3; n/2. Three regions of solutions now exist. The number of possible recombination's that can exist is 3! = 6. At this point there are nine solutions in the SP_{struct} . The general representation is given as:

$$k \ge 1 + 2! + 3! + \dots + 2! \tag{1}$$

where z is the total number of permutations possible and k is P_{size}/n .

The second part of SP_{struct} is made from solution in descending order $x_{desending} = \{n,, 2, 1\}$. A similar approach is used for generating the rest of the possible permutations. The end result is that *n* separate populations exist and are used independently by the underlying heuristic.

1.2 Solution Dynamics

A solution represented as $x = \{x_1, x_2, ..., x_n\}$, where *n* is the number of variables, within a population has a number of attributes. Usually the most visible is its fitness value, by which it is measured within the population. This approach is not so viable in order to measure

Table 1: Solution Parameters

Parameter	Description	Activity
Deviation	Measure of deviation	Control
Spread	Alignment of solution	Control
Life	Generation cycles	Selection
Offspring	No. of offspring's	Selection

	Table 2	: Spread	genera	lization
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Spread	Generalization
> 0	Forward spread
0	Even spread
< 0	Reverse spread

the diversity of the solution in the population. In retrospect, a single solution is assigned a number of attributes for measure, as given in Table 1. The most important attribute is the *deviation* (the difference between successive values in a solution). Since we are using only permutative solutions, deviation or *ordering* of the solution is important. This is due to the fact that each value in the solution is unique. Each value in the solution has a unique footprint in the search space. The formulation for deviation is given as:

$$\delta = \left(\frac{\sum_{i=1}^{n-1} |x_i - x_{i+1}|}{n}\right) x_i \in \{x_1, x_2, ..., x_n\}$$
(2)

Spread of a solution gives the alignment of the solution. Each permutative solution has a specific ordering, whether it is *forward* aligned or *reverse* aligned. Whereas deviation measures the distance between adjacent solutions, spread is the measure of the hierarchy of subsequent solutions given as:

$$\partial = \begin{cases} +1 & if (x_{i+1} - x_i) \ge 1\\ -1 & if (x_{i+1} - x_i) \le 1\\ & i \in \{1, 2, \dots, n\} \end{cases}$$
(3)

The generalisation of *spread* is given in Table 2. *Life* is the number of generations the solution has survived in the population and *Offspring* is the number of viable solutions that have been created from that particular solution. These two variables are used for evaluating the competitiveness of different solutions.

1.3 Clustering

Within the population, certain solutions exhibit attracting features. These points are usually local optima regions, which draw the solutions together. The approach utilized is to subdivide the population in clusters, each cluster a distinct distance from another. Two controlling parameters are now defined which control the clusters.

Cluster Attractor C_A : The distance that each segment of solution has to differ from each other. The C_A is given in (4).

$$C_A \in [0.1, 1+)$$
 (4)

	D	0 1		0	T .
Solution	Dev	Spread	Clust	C_A	Fitness
12345678910	0.9	+9	1	1.2	1592
1 2 5 6 9 10 3 4 7 8	2.1	+7	2	1.1	1559
10987654321	0.9	-9	1	1.2	1567
10965218743	2.1	-7	2	1.1	1547
64823915710	3.7	+3	3	0.4	1765
94375210168	4.1	-1	4	-	1788
87413652109	2.5	-3	2	1.1	1678
25791810364	3.6	+3	3	0.4	1686
61397105284	3.6	-1	3	0.4	1654
59268317104	3.9	+1	4	-	1545
	90.13379				

Table 3: Illustrative example

Within the population indexed by the *deviation*, solutions with similar deviation are clustered together, and each cluster is separated by at least a single C_A as seen in (5).

$$\begin{array}{l} (\delta_1, \delta_2, \dots, \delta_i) \stackrel{C_A}{\leftrightarrow} (\delta_{i+1}, \delta_{i+2}, \dots, \delta_{2i}) \stackrel{C_A}{\leftrightarrow} \\ \dots \stackrel{C_A}{\leftrightarrow} (\delta_{3i+1}, \delta_{3i2}, \dots, \delta_{4i}) \end{array}$$
(5)

An illustrative example is presented to showcase how this approach works. Assume a group of solutions as presented in Table 3.

Each solution is evaluated for its deviation and spread as given in columns 2 and 3. Column 4 gives the cluster to which the solution belongs, and column 5 gives the value of C_A by which each cluster is separated from each other. The graphical representation is given in Fig. 1.

The second controlling factor is the *Cluster Edge* C_E . Whereas C_A is the mapping of individual solutions, C_E is the measure of the entire population. C_E is the measure of the deviation of the fitness of the population and to prevent the population from stagnating to any fitness minima.



Figure 1: Graphical representation of population

Table 4: Selection criteria

Variables	Criteria
Fitness	Improves clusters best solution
C_A	Increases the value of C_A
C_E	Decreases

Table 5: Deletion criteria							
	Variables	Criteria					
	Life	High					
	Offspring	Low					
	C_A	Decreases					

1.4 Selection and Deletion

Selection of the next generation is based on a tier-based system. If the new solution improves on the global minima, it is then accepted in the solution. Otherwise, competing clusters jockey for the new solution. Initially the solution is mapped for its deviation. This deviation is then mapped to the corresponding cluster.

Within the cluster, the placement of the solution is evaluated. If the new solution corresponds to an existing solution, or reduces the threshold C_A value of the cluster, then it is discarded.

The solution is accepted if it improves on the C_A value of the cluster (hence improving diversity) and also to some extent keeps the balance of the C_E . If the cluster has less than average solutions, then the new solution is admitted.

Table 4 gives the selection criteria. Once the solution is added to the cluster, another solution can be discarded. This solution is usually elected from the middle placed solutions in the cluster, whose fitness is not in the top 5% of the population. If no such solutions exist, then the average rated solution is removed. Solution with high *Life* and low *Offspring* are discarded, since they are considered dormant within the cluster.

Table 5 gives the deletion criteria.

2 DIFFERENTIAL EVOLUTION

Differential Evolution (DE) given by Price (1999), is the heuristic which was used in conjunction with the clustered population. DE uses a vector perturbation methodology for crossover.

Each solution is visualized as a vector in search space. A new vector is created by the combination of four unique vectors. A schematic of DE applied to clustering is given in Fig. 2.

There are ten working strategies for DE, but the one selected for implementation is the DE/rand/2/bin represented as in (6):

$$U_{i,G+1} = x_{best,G} + F \cdot (x_{j,r_1,G} - x_{j,r_2,G} - x_{j,r_3,G} - x_{j,r_4,G})$$
(6)

This strategy was selected since it maps to the four unique clusters in the SP. The best solution is selected from the entire SP based on fitness value. Then, each random solution is selected from each distinct cluster. Again

1. Input: $D, G_{\max}, NP \ge 4, F \in (0, 1+), CR \in [0,1]$, and initial bounds: $\vec{x}^{(lo)}, \vec{x}^{(lo)}$. 2. While $G < G_{\max}$ 3. Mutate and recombine: 3.1 $r_1, r_2, r_3, r_4 \in \{1, 2, ..., P_{size}\}$, randomly selected from each cluster 3.2 $j_{rand} \in \{1, 2, ..., D\}$, randomly selected once each i3.3 $\forall j \le D, u_{j,i,G+1} = \begin{cases} x_{bet,G} + F \cdot (x_{j,e_i,G} - x_{j,e_3,G} - x_{j,e_3,G}) \\ if (rand_j[0,1] < CR \lor j = j_{rand}) \end{cases}$ 4. Select Criteria G = G + 1

Figure 2: DE selection

the selected values are checked for opposing *spread*. If the spread is identical, then a second round of selection occurs. A schematic is given in Fig. 3. The selection



Deviation solution space

Figure 3: DE selection

of the cluster is random, so r_1 can be selected from any cluster with no preference. These values are subtracted given as $x_{j,r_1,G} - x_{j,r_2,G} - x_{j,r_3,G} - x_{j,r_4,G}$. The resulting value is multiplied by the scaling factor F and added to the best solution as given in Fig. 4. The resulting value is only accepted in the new solution if a generated random number is below the given threshold provided by the controlling parameter of CR. This procedure provides added stochasticity to the heuristic.

As can be envisioned, the resulting value obtained is a real number. The repairment routine of Onwubolu and Davendra (2009) is used for repairment of the solutions.

Since it is also possible to obtain identical values in the solution after DE crossover, the repairment routine is applied to repair the solutions.



Deviation solution space

Figure 4: DE crossover

3 GENERAL TEMPLATE

Collating all the piecewise explanation, a general generic template is now described.

- 1. *Initialize*: Assign the problem size n, population size P_{size} , sub population sizes $SP_{struct} SP_{rand}$, and the control parameters of C_A and C_E .
- 2. Generate: Randomly create SP_{rand} , halves the size of P_{size} , and then structurally create SP_{struct} . These two form the basis of the population.
- 3. Calculate: Calculate the deviation and spread of each solution. Taking deviation values, configure the population into four clusters. The minimal separation value between the clusters is assigned as C_A . Taking the entire SP, the standard deviation of the fitness is computed. This is labelled as the C_E .
- 4. Generation
 - (a) DE is applied to each SP in turn.
 - (b) The new solution is calculated for its *deviation* and *spread*.
 - (c) Using the selection criteria, the solution is placed within the cluster corresponding to its deviation. If replicated solutions exist, then it is discarded. Selection is based on *fitness* and the move of the C_A and C_E .
- 5. *Re-calculation:* The SP is re-calculated for its cluster boundaries.
- 6. Dynamic clustering: If the value of C_A has decreased, then the boundary solutions are reconfigured. The C_E value is calculated for the new population.

4 FLOW SHOP SCHEDULING

One of the common manufacturing tasks is *scheduling*. Often in most manufacturing systems, a number of tasks have to be completed on every *job*. Usually all these jobs have to follow the same route through the different *machines*, which are set up in a series. Such an environment is called a *flow shop* (FSS) Pinedo (1995).

The standard three-field notation Lawler et al. (2006) used is that for representing a scheduling problem as $\alpha |\beta| F(C)$, where α describes the machine environment, β describes the deviations from standard scheduling assumptions, and F(C) describes the objective C being optimised. This research solves the generic flow shop problem represented as $n/m/f||F(C_{\text{max}})$.

Stating these problem descriptions more elaborately, the minimization of completion time (makespan) for a flow shop schedule is equivalent to minimizing the objective function \Im :

$$\Im = \sum_{j=1}^{n} C_{m,j} \tag{7}$$

s.t.
$$C_{i,j} = \max(C_{i-1,j}, C_{i,j-1}) + P_{i,j}$$
 (8)

where $C_{m,j}$ = is the completion time of job j, $C_{1,1} = k$ (any given value), $C_{i,j} = \sum_{k=1}^{j} C_{1,k}$; $C_{j,i} = \sum_{k=1}^{i} C_{k,1}$, $i \Rightarrow$ machine number, $j \Rightarrow$ job in sequence, $P_{i,j} \Rightarrow$ processing time of job j on machine i. For a given sequence, the mean flow time, $MFT = \frac{1}{n} \sum_{i=1}^{m} \sum_{j=1}^{n} c_{i,j}$, while the condition for tardiness is $c_{m,j} > d_j$. The constraint of Equation 8 applies to these two problem descriptions.

5 EXPERIMENTATION

The first sets of Flowshop scheduling benchmark problems are Car Carlier (1978), Rec Reeves (1995) and Hel Heller (1960) benchmark sets. A total of 31 instances exist, each of varying size and difficulty Ponnambalam et al. (2001).

Comparison is done with other published heuristics on the same problem instances. Comparison of the DE_{Clus} heuristics is done with the Improved Genetic Algorithm (IGA) and Multiagent Evolutionary Algorithm (MAEA) Hu et al. (2006) and the Hybrid Genetic Algorithm (H-GA) and Othogonal Genetic Algorithm (OGA) of Tseng and Lin (2006). The results are given in Table 6.

The results of DE were obtained from Davendra and Onwubolu (2007). In 11 instances, the optimal value was obtained, and on average the percentage increase was below 1%. Using clustering, DE_{clus} markedly improves all the solutions. This is clearly seen in the large problems sizes of 50 jobs and more. The improvement is clearly in excess of 1.5%.

Table 7: Comparison of Taillard Instances

	PSC	O_{spv}	DE_{sp}	v + ex	D	E	DE	clus
Problem	Δ avg	Δ std						
20x5	1.71	1.25	0.69	0.64	0.98	0.66	0.55	0.71
20x10	3.28	1.19	2.01	0.93	1.81	0.77	1.32	0.98
20x20	2.84	1.15	1.85	0.87	1.75	0.57	0.98	1.32
50x5	1.15	0.7	0.41	0.37	0.4	0.36	0.33	0.76
50x10	4.83	1.16	2.41	0.9	3.18	0.94	3.13	0.77
50x20	6.68	1.35	3.59	0.78	4.05	0.65	3.67	0.56
100x5	0.59	0.34	0.21	0.21	0.41	0.29	0.38	0.54
100x10	3.26	1.04	1.41	0.57	1.46	0.36	1.31	0.32
100x20	7.19	0.99	3.11	0.55	3.61	0.36	2.23	0.45
200x10	2.47	0.71	1.06	0.35	0.95	0.18	0.69	0.54

In general comparison with published results, the clustered approach of DE_{clus} is one of the top two performing heuristics. MAEA approach is the best comparative heuristic and in comparison with DE_{clus} , even though MAEA obtains more optimal solutions, DE_{clus} , performs more consistently in large problems.

The second set of benchmark problems is referenced from Taillard (1993). These sets of problems have been extensively evaluated by Reeves and Yamada (1998). This benchmark set contains 120 particularly hard instances each of 10 different size, selected from a large number of randomly generated problems.

The results are tabulated as quality solutions with the percentage relative increase in makespan with respect to the upper bound provided by Taillard (1993). To be specific the formulation is given as:

$$\Delta_{avg} = \frac{(H-U) \times 100}{U} \tag{9}$$

where H denotes the value of the makespan that is produced by the utilized algorithm and U is the upper bound or the lower bound as computed.

Comparison is done with the results obtained for DE_{clus} with those produced by Particle Swarm Optimization PSO_{spv} and DE with local search $DE_{spv+exchange}$ as in Tasgetiren et al. (2004b) and Tasgetiren et al. (2004a) and compared in Table 7.

 DE_{clus} obtains better results in the instances of (20x5, 20x10, 20x20, 50x5,100x10, 100x20, 200x10) and $DE_{spv+exchange}$ performing best in the remaining (50x10, 50x20, 100x5) instances. The advantage of $DE_{spv+exchange}$ is the fact that it employs local search, whereas DE_{clus} is employing 2-opt local search as given in Onwubolu and Davendra (2009).

DE with clustering produces better results than DE without clustering, validating the approach of embedding population dynamics.

6 ANALYSIS AND CONCLUSION

A detailed operational analysis of the heuristic is now presented. A sample program output is presented to illustrate the heuristic behaviour during experimentation. Fig. 5 and Fig. 6 gives the first and final populations mapped on the deviation space.

Name	n x m	Cost	H-GA	OGA	IGA	MAEA	DE	DE_{Clus}
Car1	11x5	7038	0	0	0	0	0	0
Car2	13x4	7166	0	0	0	0	0	0
Car3	12x5	7312	0	0	0	0	0	0
Car4	14x4	8003	0	0	0	0	0	0
Car5	10x6	7720	0	0	0	0	0	0
Car6	8x9	8505	0	0	0	0	0	0
Car7	7x7	6590	0	0	0	0	0	0
Car8	8x8	8366	0	0	0	0	0	0
Rec01	20x5	1247	0	0.04	0	0	0	0
Rec03	20x5	1109	0	0	0	0	0	0
Rec05	20x5	1242	0.08	0.21	0	0	0	0
Rec07	20x10	1566	0	0.79	0	0	0	0
Rec09	20x10	1537	0	0.35	0	0	0	0
Rec11	20x10	1431	0	0.91	0	0	0	0
Rec13	20x15	1930	0.52	1.08	0.62	0	0.45	0.31
Rec15	20x15	1950	0.92	1.23	0.46	0	0.32	0.28
Rec17	20x15	1902	1.26	2.08	1.73	0	0.29	0.28
Rec19	30x10	2093	0.38	1.76	1.09	0.28	0.42	0.338
Rec21	30x10	2017	0.89	1.64	1.44	0.44	0.39	0.38
Rec23	30x10	2011	0.45	1.9	0.45	0.44	0.21	0.21
Rec25	30x15	2513	1.03	2.67	1.63	0.43	0.32	0.29
Rec27	30x15	2373	1.18	2.09	0.8	0.56	0.42	0.27
Rec29	30x15	2287	1.05	3.28	1.53	0.78	0.61	0.34
Rec31	50x10	3045	0.56	1.49	0.49	0.1	0.7	0.32
Rec33	50x10	3114	0	1.87	0.13	0	0.84	0.28
Rec35	50x10	3277	0	0	0	0	0.91	0.27
Rec37	75x20	4951	2.54	3.41	2.26	2.72	1.32	0.33
Rec39	75x20	5087	1.79	2.28	1.14	1.61	1.56	0.29
Rec41	75x20	4960	2.82	3.43	3.27	2.7	1.98	0.28
Hel01	100x10	513	-	-	-	0.38	2.1	0.53
Hel02	20x10	135	-	-	-	0	1.97	0

Table 6: Comparison of clustered heuristics with other published heuristics



Figure 5: DE_{clust} initial population

The evident feature of the two plots is that the diversity of the solutions increased over the generations. Another feature is that separate search spaces were explored since the deviation value increased over the generations.

The second controlling parameter of C_E , which controls the grouping of the population, is given in Fig. 7. As seen from 7, there is a general decline of C_E within DE_{clust} . This is evident for a major migration of the cluster.

The history of the best solution is presented in Fig. 8. Clustering improves solution diversity, however the importance of C_E can be easily seen when comparing the two plots of C_E in Fig. 7 and best solution in Fig. 8. A



Figure 6: DE_{clust} final population

correlation is observed between the two plots, since any major activity in C_E has a flow on impact to the best individual. The explanation is that once the cluster drifts into new solution spaces, a rapid divergence occurs, which leads to possibly discovery of new optimal solutions.

Once the local space is searched, a different directional search occurs, which generally results in an increase of the value of C_E , as observed from the two different plots.

Another unique feature of the experimentation as the fact that approximately 45% of solutions were obtained from the structured population. This validates the approach of utilising a structured initial population along-side a random population.



Figure 7: $DE_{clust} C_E$ values over the generations



Figure 8: Best solution history of DE_{clust}

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A PRACTICAL O-D MATRIX ESTIMATION MODEL BASED ON FUZZY SET THEORY FOR LARGE CITIES

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KEYWORDS

O-D matrix estimation, Traffic counts, Fuzzy theory.

ABSTRACT

Estimation of the origin-destination trip demand matrix (O-D) plays a key role in travel analysis and transportation planning and operations. Many researchers have developed different O-D matrix estimation methods using traffic counts, which allow simple data collection as opposed to the costly traditional direct estimation methods based on home and roadside interviews.

In this paper, a new fuzzy O-D matrix estimation model (FODMEM) is proposed to estimate the O-D matrix from traffic count. A gradient-based algorithm, containing a fuzzy rule based approach to control the estimated O-D matrix changes, is proposed to solve FODMEM.

Since link data only represents a snapshot situation, resulting in inconsistency of data and poor quality of the estimated O-D's, the proposed method considers link data as fuzzy values that vary within a certain bandwidth. An equilibrium based fuzzy assignment method is proposed to assign the estimated O-D matrix, which causes the assigned volumes to be fuzzy numbers. The shortest path algorithm of the proposed method is similar to the Floyd-Warshall algorithm, and we call it the Fuzzy Floyd-Warshall Algorithm (FFWA). We introduce a new fuzzy comparing index to compare and estimate the distance between the assigned and observed link volumes and the model is formulated based on this index. FODMEM is implemented in Mashhad city in Iran. Real data obtained from Mashhad Comprehension Transportation Study (MCTS) are used in this study and results are presented to show high capability of FODMEM to estimate O-D matrix in large networks.

INTRODUCTION

Obtaining the origin-destination (O-D) matrix by conventional methods takes a considerable amount of time, money, and manpower, while gathering traffic volume data for the links of the transportation network is easy. Recently, a variety of analytic models has been developed to establish O-D trip matrices based on traffic counts along with other information. Although O-D matrix estimation models from traffic counts are different in formulation, they are similar in that their implementation is extremely difficult in largescale networks. Another important problem is the inconsistency among link-count data that results in poor quality of the estimated O-D's and even nonconvergence of the solution algorithm. Data inconsistency occurs due to diverse reasons, such as counting error and the deriver's behaviour. Some researchers tried to solve this problem by using a set of "Fuzzy Weights" for each piece of inconsistent data (Xu and Chan 1993). They considered the link counts as imprecise values, so they proposed to survey link volumes more than once and computed fuzzy weights for every set of link counts.

The traffic assignment methods utilized in the above O-D estimation models, such as equilibrium and proportional based, consider the user's route choice as a crisp and precise process. Some research has demonstrated that the common equilibrium based assignment methods cannot correctly reproduce real traffic volumes. It is indicated that real assigned traffic flow might not certainly converge to the userequilibrium. In other words, travel times used in routes have salient differences from the lowest route travel time (Jan and Ridwan 1994). As a result, it should be realized that common equilibrium and stochastic assignment models do a poor job of accounting for imprecision and uncertainty in the user's route choice behavior. Recently, some assignment models based on fuzzy theory have been proposed, but these models have not been widely used in the O-D estimation problem. Some researchers proposed a fuzzy inference based assignment algorithm in the O-D matrix estimation problem (Harikishan and Partha 1998). They applied an entropy model previously developed in the upper level of the O-D estimation problem.

In this paper, we use a new fuzzy approach to propose equilibrium based O-D matrix estimation model. We implement this model in Mashhad City, one large city in Iran. This model has a bi-level structure, and the fuzzy approach is applied in both the upper and lower levels.

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THE PROPOSED FUZZY O-D MATRIX ESTMATION MODEL (FODMEM)

Here, we propose the fuzzy O-D matrix estimation model (FODMEM). The model is formulated as an optimization problem. The objective function tries to minimize the fuzzy distance between the assigned and observed link volumes based on a new fuzzy index I_1^c :

min
$$Z(q) = \frac{1}{2} \sum_{a \in \hat{A}} \left(1 - I_1^c \left(\tilde{\hat{x}}_a \right) \right)^2$$
 (1)

s.t.
$$\tilde{x} = assign(q)$$
 (2)

q : Trip demand matrix

assign(q): Fuzzy traffic assignment

 \hat{A} : The observed links set

The observed link volume is defined as a fuzzy value:

$$\widetilde{\hat{x}} = \left(\hat{x}^L, \hat{x}, \hat{x}^R \right) \tag{3}$$

where \hat{x} is the crisp value of observed link volume, and $\hat{x}^{L} = \hat{x} (1 - \beta_{l})$ and $\hat{x}^{R} = \hat{x} (1 + \beta_{r})$ are the lower and upper boundaries. β_{l} and β_{r} are experimental values and represent the degree of imprecision in link counts, which can be obtained based on expert knowledge or observation of daily traffic variation of each link in a specific time period.

The assigned fuzzy link volumes \tilde{x} is formulated as below:

$$\widetilde{x} = \left(x^{L}, x, x^{R}\right) \tag{4}$$

where \tilde{x} is the fuzzy link volume, x is the assigned link volume, and $x^{L} = x(1 - \alpha_{l})$ and $x^{R} = x(1 + \alpha_{r})$ are the lower and upper boundaries. The parameter α_{r} is the link degree of saturation, and α_{l} is an experimental value. These parameters can be specified through different approaches, such as interviewing, using expert knowledge or simulation. $I_{1}^{c}(\tilde{x}_{a})$ is the proposed fuzzy comparison index between the fuzzy observed link volume \tilde{x}_{a} and the fuzzy assigned link volume \tilde{x}_{a} in link a. This index is computed as below:

$$I_1^c\left(\widehat{\tilde{x}}_a\right) = \frac{x_a^R - \hat{x}_a^L}{\left(\widehat{x}_a - \widehat{x}_a^L\right) + \left(x_a^R - x_a\right)}, \quad -\infty \le I_1^c \le \infty$$
(5)

Where:

$$I_1^c\left(\widetilde{\hat{x}}_a\right) = I_1^c\left(\widetilde{x}_a\right) = 1 \Leftrightarrow \widetilde{\hat{x}}_a = \widetilde{x}_a$$

$$I_1^c(\widetilde{\hat{x}}_a) < 1 \Longrightarrow \widetilde{\hat{x}}_a > \widetilde{x}_a, \quad I_1^c(\widetilde{\hat{x}}_a) > 1 \Longrightarrow \widetilde{\hat{x}}_a < \widetilde{x}_a$$

Figure 1 illustrates the schematic diagram of this index for two fuzzy number "M" and "N", which is defined as the height of cross point of $[M,\infty)$ and $(-\infty, N]$:

$$\mu_{(-\infty,N]}(x) = \frac{n-x}{n^R - n} , \forall x$$
(6)

$$\mu_{[M,\infty)}(x) = \frac{x - m^L}{m - m^L} , \forall x$$
(7)



Figures 1: The fuzzy comparison index $I_1^c(M)$

The lower level of problem assign(q) includes a new fuzzy traffic assignment model (Shafahi and Ramezani 2007), resulting in the assigned fuzzy link volumes \tilde{x} . Shafahi and Ramezani assumed that the user's decision-making process in route choice is based on their perceived travel time (PTT), which is presented as a triangle fuzzy number:

$$\widetilde{t} = \left(t^L, t^C, t^R\right) \tag{8}$$

where \tilde{t} is the fuzzy link travel time, t^{C} is the assigned link travel time, and t^{L} and t^{R} are the lower and upper

boundaries. The route choice decision-making process in this model is based on the fuzzy ranking method (Dubois and Prade 1983). Shafahi and Ramezeni chose the index I_3 as the better ranking criterion in the selection of the best path and assigning traffic (Shafahi and Ramezani 2007). The computation formula of the index I_3 for comparing two fuzzy link travel times \tilde{t}_1 and \tilde{t}_2 is equal to:

$$I_{3}(\tilde{t}_{1}) = \frac{t_{2}^{R} - t_{1}}{\left(t_{1}^{R} + t_{2}^{R}\right) + \left(t_{1} + t_{2}\right)}$$
(9)

When the index I_3 values for two fuzzy numbers are equal, these numbers have no differences. Shafahi and Ramezani demonstrated that two fuzzy numbers $\tilde{t_1}$ and $\tilde{t_2}$ are equal if:

$$I_{3}(\widetilde{t}_{1}) = I_{3}(\widetilde{t}_{2}) = 0.5 \Leftrightarrow \widetilde{t}_{1} = \widetilde{t}_{2}$$

$$(10)$$

We improve Shafahi and Ramezani's fuzzy Shortest Path Algorithm (FSPA), which is similar to the Dijkstra algorithm and propose a more efficient and faster approach based on the Floyd-Warshall shortest path algorithm (FWA). This algorithm simultaneously finds the shortest path between all nodes. In the approach, Similar to the FSPA algorithm, we use the index I_3 described above to compare link PTTs and to choose the shortest path, and call it "Fuzzy Floyd-Warshall Algorithm (FFWA)". To run FFWA: S: The set of all nodes,

 $\widetilde{d}(i, j)$: The fuzzy distance (fuzzy travel time) of the shortest path between two nodes $i, j \in S$,

 $\tilde{l}(i, j)$: The fuzzy length of the link between two nodes i and j. The link length between i and i is defined to be 0, and the length of two nodes without any direct links between them is assumed to be ∞ .

min : The function computes the minimum of the fuzzy lengths according to index I_3 .

FFWA is as follows:

Step 1- Initialization

Set: $\widetilde{d}(i, j) = \widetilde{l}(i, j)$, for all i, j.

Step 2- Induction

For all
$$k \in S$$

For all i, j
Set: $\widetilde{d}(i, j) = \min \left| \widetilde{d}(i, j), \widetilde{d}(i, k) + \widetilde{d}(k, j) \right|$

Set: $\tilde{d}(i, j) = \min[\tilde{d}(i, j), \tilde{d}(i, k) + \tilde{d}(k, j)]$ Fuzzy Equilibrium Principle: If "M" and "N" are assumed to be two used paths between a distinct origin and destination and "K" is an unused path between that origin and destination, then the following equations hold(Shafahi and Ramezani 2007):

$$I_3(M) = I_3(N) = 0.5 \tag{11}$$

$$I_3(K) \le 0.5$$
 (12)

The fuzzy assignment algorithm is an incremental assignment, so that it can be called Fuzzy Incremental Traffic Assignment algorithm (FITA). Assuming that the travel time function of the link "a" is $t_a(x_a)$, the trip demand for origin-destination *rs* is q_{rs} , and *N* is the repetition number of the incremental algorithm, then the assignment algorithm is:

Step 0 (Initialization) - Given N, α_l , α_r , and δ (δ =a small value, say 0.001), set:

$$n = 1$$
, $t_a = t(0)$, $t_a^R = t(0) + \delta$, $t_a^L = t(0) - \delta$

Step 1- For all O-D pairs rs, find the shortest paths and assign $\frac{q_{rs}}{N}$ to the shortest paths. Step 2- Update link travel times according to the volumes assigned in the previous step:

$$t_a = t_a(x_a), \ t_a^R = t_a[(1+\alpha_r)x_a], \ t_a^L = t_a[(1-\alpha_l)x_a]$$

 x_a = Assigned volume to link "a"

Step 3 (stop criterion) - if n = N stop, otherwise set n = n + 1 and go to step 1.

Ramezani proved the convexity of the fuzzy assignment model (Ramezani 2007), so equation (1) includes a convex problem that ensures the uniqueness of the problem solution in the lower level. However, there is an infinite number of possible matrices that might result in the observed volumes, so similar to conventional O-D estimation models, we consider an original O-D matrix \hat{q} from past demand studies to guide the output solutions and expect the resulting matrix to closely resemble the original matrix. We use the gradient method as an efficient way to minimize deviation from the starting solution. Thus, we can obtain the most reliable O-D matrix among all possible matrices, which is near the original demand matrix and reproduces the observed link volumes (Spiess 1990). Here, we improve upon this method for our fuzzy approach.

Based on the gradient method, the relative change in demand q can be written as:

$$q_{rs}^{l+1} = \begin{cases} \hat{q}_{rs} & ,l=0\\ q_{rs}^{l} \left[1 - \lambda^{l} \left(\frac{\partial z(q)}{\partial q_{rs}} \right)_{q_{rs}^{l}} \right] & ,l=1,2,3... \end{cases}$$
(13)

where \hat{q}_{rs} and q_{rs}^{l} denote the original matrix and the adjusted demand matrix in step l for origin-destination pairs rs. This approach implies that the O-D pairs without trip demand would not be affected by the adjustment and zeros will be preserved. The parameter λ^{l} is the step length and has to be chosen small enough to ensure that the path followed by q_{rs}^{l} is sufficiently close to the true gradient path. The parameters $\frac{\partial z(q)}{\partial q_{rs}}$ and λ^{l} have to be computed in the adjustment process. The relationship between link volumes and path flows in the fuzzy equilibrium assignment is expressed as below:

$$\widetilde{x}_{a} = \sum_{rs} \sum_{k} \widetilde{f}_{k}^{rs} \delta_{a,k}^{rs} , a \in A$$
(14)

 $k \in K_{rs}$ is the set of paths used for each origindestination rs. An expression for the gradient $\frac{\partial z(q)}{\partial q_{rs}}$ is easily determined if the path probabilities are used instead of path flows, as shown:

$$P_k = \frac{f_k^{rs}}{q_{rs}} , k \in K_{rs}, rs \in RS$$
(15)

So equation (14) can be rewritten as:

$$x_a = \sum_{rs} q_{rs} \sum_k \delta_{a,k}^{rs} P_k \quad , a \in A$$
 (16)

For simplification, we use f_k^{rs} as the center of fuzzy path flow \tilde{f}_k^{rs} and x_a as the center of the assigned link volume \tilde{x}_a in (15) and (16).

We can compute $\frac{\partial z(q)}{\partial q_{rs}}$ using the chain rule:

$$\frac{\partial z(q)}{\partial q_{rs}} = \frac{\partial z(q)}{\partial I_{1}^{c}(\hat{x}_{a})} \times \frac{\partial I_{1}^{c}(\tilde{x}_{a})}{\partial x_{a}} \times \frac{\partial x_{a}}{\partial q_{rs}}$$
$$\frac{\partial z(q)}{\partial q_{rs}} = \sum_{k \in K_{RS}} P_{k}^{rs} \sum_{a \in \hat{A}} \delta_{a,k}^{rs} \frac{\hat{x}_{a}(\beta_{r} + \alpha_{r})(x_{a} - \hat{x}_{a})}{(\beta_{r}\hat{x}_{a} + \alpha_{r}x_{a})^{3}} \quad (17)$$

The other parameter we need to implement in the gradient method is the step length λ^{l} . Choosing very small values for this parameter results in a more precise gradient path, but leads to an increase in the required number of steps to reach the optimal solution. Therefore, by solving the one-dimensional subproblem illustrated below, the optimal step lengths λ^{*} can be found:

min
$$Z(\lambda) = \frac{1}{2} \sum_{a \in A'} \left(1 - I_1^c \left(\widehat{\widetilde{x}}_a \right) \right)^2$$
 (18)

s.t.
$$\widetilde{x}(\lambda) = assign\left(q_{rs}\left(1 - \lambda \frac{\partial z(q)}{\partial q_{rs}}\right)\right)$$
 (19)

The parameter $x_a(\lambda)$ as the center of fuzzy value $\tilde{x}_a(\lambda)$ is substituted instead of the assigned volume center x_a in (19). This parameter is computed below using the assumption that path probabilities do not change during the corresponding iteration:

$$x_{a}(\lambda) = \sum_{rs} \left[q_{rs} \left(1 - \lambda \frac{\partial z(q)}{\partial q_{rs}} \right) \right] \sum_{k} \delta_{a,k}^{rs} P_{k}$$
(20)

Also, we obtain:

$$x'_{a} = \frac{\partial x_{a}(\lambda)}{\partial \lambda} = -\sum_{rs} q_{rs} \frac{\partial z(q)}{\partial q_{rs}} \left(\sum_{k} \delta^{rs}_{a,k} P_{k} \right)$$
(21)

which yields:

$$x_a(\lambda) = x_a + \lambda x_a' \tag{22}$$

Because x_a and x'_a are independent of λ , the optimal step length can be found by computing the zero of the derivative. The derivative is again obtained by applying the chain rule:

$$\frac{\partial z(\lambda)}{\partial \lambda} = \frac{\partial z(\lambda)}{\partial I_1^c} \times \frac{\partial I_1^c}{\partial \lambda}$$
$$\frac{\partial z(\lambda)}{\partial \lambda} = \sum_{a \in \hat{A}} \frac{x'_a \hat{x}_a(\alpha_r + \beta_r) [(x_a + \lambda x'_a) - \hat{x}_a]}{[\beta_r \hat{x}_a + \alpha_r (x_a + \lambda x'_a)]^3} = 0 \quad (23)$$

assuming $\alpha_r = \beta_r$:

$$\lambda^* = \frac{\sum\limits_{a \in \hat{A}} \frac{x'_a(\hat{x}_a - x_a)}{\hat{x}_a^2}}{\sum\limits_{a \in \hat{A}} \left(\frac{x'_a}{\hat{x}_a}\right)^2}$$
(24)

subject to:

$$\hat{q}_{rs} > 0$$
 with $rs \in RS$, for all $\lambda \frac{\partial z(q)}{\partial q_{rs}} \le 1$ (25)

By using equations (17) and (24), we can solve for all unknowns in (13).

An Expert Based Fuzzy Control Rule

Here, we propose an initiative fuzzy rule based approach to control the O-D matrix changes and to enter expert knowledge in the estimation process. First, the original O-D matrix elements are clustered into tree clusters: c_1 , c_2 , and c_3 as "Small", "Medium", and "Large" O-D demand values, using C-means fuzzy clustering method (Zimmermann 1996), and then we define the maximum allowable change of demand values assigned to each cluster using a fuzzy rule base. This method results in controlling and limiting the estimated O-D matrix, preventing unreasonable changes during algorithm iterations.

By testing different membership functions for elements of clusters, we choose the "Gaussian Function" as the best fitting one. In the next step, we define three experimental fuzzy sets: ac_1 (Large), ac_2 (Medium), and ac_3 (Small) as maximum allowable changes to O-D demand values, which are shown in figure 2. There are no restrictions considered to the minimum allowable changes. Therefore, the membership functions presented in Figure 2 are in a non-symmetric formation.



Figures 2: Fuzzy membership of maximum allowable change of O-D demand values

The fuzzy membership functions are:

$$\mu_{ac_1}(x) = \begin{cases} 3-x & ,2 \le x \le 3\\ 0 & ,otherwise \end{cases}$$
(26)

$$\mu_{ac_2}(x) = \begin{cases} 4 - 2x & , 1.5 \le x \le 2\\ 0 & , otherwise \end{cases}$$
(27)

$$\mu_{ac_3}(x) = \begin{cases} 6-4x & , 1.25 \le x \le 1.5 \\ 0 & , otherwise \end{cases}$$
(28)

Finally, we define the fuzzy rule base including three fuzzy rules as follows:

If
$$\hat{q}_{rs}$$
 is "Small", then $\left(\frac{q_{rs}}{\hat{q}_{rs}}\right)_{max}$ is "Large" (29)

If
$$\hat{q}_{rs}$$
 is "Med", then $\left(\frac{q_{rs}}{\hat{q}_{rs}}\right)_{max}$ is "Med" (30)

If
$$\hat{q}_{rs}$$
 is "Large", then $\left(\frac{q_{rs}}{\hat{q}_{rs}}\right)_{max}$ is "Small" (31)

We assume that as the demand increases (in developed zones), the relevant allowable change decreases and as the demand decreases (in developing zones), the relevant allowable change increases.

In the final step, the results are combined and defuzzified and the maximum allowable change of O-D demand values σ_{rs} is computed as a crisp number. We use the center of gravity (COG) method as the most popular defuzzification method (Zimmermann 1996), which is computed by the following equation:

$$\left(\frac{q_{rs}}{\hat{q}_{rs}}\right)_{\max}^{crisp} = \sigma_{rs} = \frac{\sum_{i=1}^{R} b_i \int_x \mu_{ac_i}(x) dx}{\sum_{i=1}^{R} \int_x \mu_{ac_i}(x) dx}$$
(32)

where *R* is the number of rules (here R = 3), b_i is the center of area of the membership function of ac_i for the i^{th} rule, and $\int_x \mu_{ac_i}(x) dx$ denotes the area under $\mu_{ac_i}(x)$. We add the constraint below to the O-D estimation model:

$$\hat{q}_{rs} > 0$$
 with $rs \in RS$, for all $\frac{q_{rs}}{\hat{q}_{rs}} \le \sigma_{rs}$ (33)

Solution Algorithm

Finally, the solution algorithm can be proposed as follows:

Step 0 (Initialization) - Given β_l and β_r (the degree of link count imprecision), set:

$$l=0 \qquad q_{rs}=q_{rs}^l=\hat{q}_{rs}$$

Step 1 - Assign the demand matrix q_{rs}^{l} by the proposed fuzzy assignment method to find the center of the assigned fuzzy volume x_{a} .

Step 2 - Find used paths K_{rs} and the center of fuzzy path flows for every $rs \in RS$. Compute the value of parameters $\frac{\partial z(q)}{\partial q_{rs}}$ and λ as below:

$$\frac{\partial z(q)}{\partial q_{rs}} = \sum_{k \in K_{RS}} P_k^{rs} \sum_{a \in \hat{A}} \delta_{a,k}^{rs} \frac{\hat{x}_a (\beta_r + \alpha_r) (x_a - \hat{x}_a)}{(\beta_r \hat{x}_a + \alpha_r x_a)^3}$$
$$\lambda^l = \frac{\sum_{a \in \hat{A}} \frac{x_a' (\hat{x}_a - x_a)}{\hat{x}_a^2}}{\sum_{a \in \hat{A}} \left(\frac{x_a'}{\hat{x}_a}\right)^2}$$

Step 3 - If constraint (25) or the demand maximum allowable change condition (33) is not satisfied, the revised value of step length is:

$$\lambda^l = \frac{\kappa_1 + \kappa_2}{2}$$

for which:

$$\kappa_{1} = \min\left[\max\left\{\frac{1-\sigma_{n}\left(\frac{\hat{q}_{n}}{q_{n}^{\prime}}\right)}{\frac{\partial z(q)}{\partial q_{n}}}\Big|q_{n} > 0, \frac{\partial z(q)}{\partial q_{n}} > 0\right\}, \max\left\{\frac{1}{\frac{\partial z(q)}{\partial q_{n}}}\Big|q_{n} > 0, \frac{\partial z(q)}{\partial q_{n}} < 0\right\}\right]$$
$$\kappa_{2} = \max\left[\min\left\{\frac{1}{\frac{\partial z(q)}{\partial q_{n}}}\Big|q_{n} > 0, \frac{\partial z(q)}{\partial q_{n}} > 0\right\}, \min\left\{\frac{1-\sigma_{n}\left(\frac{\hat{q}_{n}}{q_{n}^{\prime}}\right)}{\frac{\partial z(q)}{\partial q_{n}}}\Big|q_{n} > 0, \frac{\partial z(q)}{\partial q_{n}} < 0\right\}\right]$$

Step 4- Determine the new values of q_{rs} using the equation below:

$$q_{rs}^{l+1} = q_{rs}^{l} \left[1 - \lambda^{l} \left(\frac{\partial z(q)}{\partial q_{rs}} \right)_{q_{rs}^{l}} \right]$$

Step 5 - Let l = l + 1 and $q_{rs} = q_{rs}^{l}$ Step 6 (stop criterion) - If $\left| 1 - I_{1}^{c} \left(\hat{\tilde{x}}_{a} \right) \right| < \varepsilon$ stop, else go to step 1.

APPLICATION OF FODMEM IN MASHHAD CITY

The FODMEM has been successfully tested by using various examples with different characteristics. An userfriendly software "FODMES" (Fuzzy O-D Matrix Estimation Software) has been produced to use the method for different examples easily.

In order to numerically illustrate the effectiveness of FODMEM in a real world networks, we implemented FODMEM for Mashhad city network, a large city in Iran. Real O-D matrix data obtained from Mashhad Comprehension Transportation Study (SCTS) in 1996 are used as original matrix in this. Mashhad city included 2.0 million people. The city is divided into 141 traffic zones and the traffic network includes 935 nodes, 2538 links and 7157 O-D pairs with non zero demand. An Origin-Destination survey with house interviewing was conducted in 1996. Data were gathered from 4% of the households and were validated by observation from different screen lines in the study area. In addition, traffic volumes of 119 links of Mashhad network are surveyed and are used as observed link volumes. Figure 3 illustrates Mashhad City network and observed links.



Figure 3: Mashhad City network and observed links

The general links travel time follows the BPR function $t(x) = t_0 \left[1 + 0.15 \left(\frac{x}{C} \right)^4 \right]$, where x, t_0 and C denote the

traffic volume, free flow travel time and practical capacity of links. All links in Mashhad network are divided into 8 classes and average values of BPR function parameters t_0 and *C* are estimated by volume-travel time observation from several links in each class as demonstrated in table 1.

Table 1: Mashhad City BPR Function Parameters

Link class	Values of BPR Function Parameters			
	t_0 (min)	C (veh/lane/hour)		
Local	1.50	350		
Collector	1.33	600		
Minor arterial- two way (CBD area)	1.20	650		
Minor arterial- two way (Non CBD)	1.20	700		
Minor arterial-one way	1.10	700		
Principal arterial (Class II)	1.00	750		
Principal arterial (Class I)	1.00	800		
Freeway	0.80	1000		

We consider 25 iterations as the stop criterion of FODMEM and 15 iterations for FITA. The parameters α_r , α_l , β_r , and β_l are assumed to be 0.2. Figure 4 shows the dispersal diagram of the observed and estimated link volumes and figure 5 shows the dispersal diagram of the estimated and original O-D matrix results of the estimated link volumes in the observed links. The *R*-squared values between the observed and estimated values (0.99 for link volume and 0.89 for O-D values) indicate that the model successfully reproduces the observed link volumes and ensures the high vicinity of the estimated O-D matrix to the original case.



Figure 4: Dispersal diagram of the observed and estimated link volume



Figure 5: Dispersal diagram of the original and estimated O-D matrix

SUMMARY AND CONCLUSION

This paper attempts to develop a fuzzy O-D estimation model FODMEM using a gradient-based algorithm to utilize more of the estimated demand matrix. The observed and assigned link volumes are defined as fuzzy numbers. This definition applies fuzzy sets to the uncertainty embedded in the driver's route choice behaviour and solves the inconsistency in link counts. A new fuzzy comparing index is proposed to evaluate link counts and assigned volumes, and to measure the fuzzy distance between them and the O-D estimation model is constructed based on this index. A gradient-based iterative algorithm is applied to solve the model. In the lower level of this model, we use an equilibrium based fuzzy assignment model (Shafahi and Ramezani 2007). We improve this model by substituting a new fuzzy shortest path algorithm FFWA based on the Floyd-Warshal algorithm, instead of using the FSPA. In order to limit unreasonable changes to the original O-D matrix, the elements of this matrix are clustered into three groups using the fuzzy clustering method and a fuzzy rule is applied to every O-D group. The proposed fuzzy rule based approach facilitates the use of expert knowledge in the model and finds a more reliable solution. Finally, Mashhad city is chosen as our case study. The results show that FODMEM can successfully find the O-D demand matrix, while reproducing the observed link volumes and the original and estimated O-D matrix closely resemble each other.

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INVESTIGATION ON OPTIMIZATION OF PROCESS PARAMETERS AND CHEMICAL REACTOR GEOMETRY BY EVOLUTIONARY ALGORITHMS

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KEYWORDS

Simulation; Optimization; Evolutionary algorithms; Differential evolution; Self-organizing migrating algorithm.

ABSTRACT

The present work aims to employ evolutionary algorithms (EAs) to optimize an industrial chemical process. A unique combination of the simplified fundamental theory and direct hands-on computer simulation is used to present the modeling of a dynamic process chemical engineering in а highly understandable way. The main aim is to use them for analysis of dynamical system behaviour, especially of a given chemical reactor. A non-linear mathematical model is required to describe the dynamic behaviour of batch process; this justifies the use of evolutionary method of the EAs to deal with this process. Two algorithms - differential evolution and self-organizing migrating algorithm are used in this investigation. Differential Evolution is an evolutionary optimization technique which is exceptionally simple, significantly faster & robust at numerical optimization and is more likely to find a function's true global optimum. SOMA is also robust algorithm in sense of global extreme searching. In this way, in order to optimize the process, the EAs code is coupled with the rigorous model of the reactor. Both algorithms (SOMA, DE) have been applied 100 times in order to find the optimum of process parameters and the reactor geometry. The results show that the EAs are used successfully in the process optimization.

INTRODUCTION

Evolutionary algorithms derived by observing the process of biological evolution in nature, have proven to be a powerful and robust optimizing technique in many cases (Gross B.; Roosen P. 1998). In computer science evolutionary computation is a subfield of artificial intelligence (more particularly computational intelligence) that involves combinatorial optimization problems (Wikipedia encyclopedia).

Since the 60s, several approaches (genetic algorithms, evolution strategies etc.) have been developed which apply evolutionary concepts for simulation and

optimization purposes. Also in the area of multiobjective programming, such approaches (mainly genetic algorithms) have already been used (Evolutionary Computation 3(1), 1–16)(Thomas Hanne 2000).

Evolutionary algorithms such as evolution strategies and genetic algorithms have become the method of choice for optimization problems that are too complex to be solved using deterministic techniques such as linear programming or gradient (Jacobian) methods. The large number of applications (Beasley (1997)) and the continuously growing interest in this field are due to several advantages of EAs compared to gradient based methods for complex problems (Ivo F. Sbalzarini, Sibylle Muller and Petros Koumoutsakos, 2000).

The optimization of dynamic process has received growing attention in recent years because it is essential for the process industry to strive for more efficient and agile manufacturing in face of saturated market and global competition (T. Backx, O. Bosgra 2000).

In chemical engineering, evolutionary optimization has been applied by the author and others to system identification (Pham and Coulter, 1995; Moros, 1996); a model of a process is built and its numerical parameters are found by error minimization against experimental data. Evolutionary optimization has been widely applied to the evolution of neural networks models for use in control applications (e.g. Li & Haubler, 1996).

In this paper, the methods of artificial intelligence by evolutionary algorithms - SOMA and DE are presented for optimizing chemical engineering processes, particularly those in which the evolutionary algorithm is used for static optimization of a chemical batch reactor to improve its parameter. Consequently, it is used to design geometry technique equipments for chemical reaction. The method was used to optimize the design of the growth chamber, and was found to be in good agreement with the observed growth rate results.

The area of reactor network synthesis currently enjoys a proliferation of contributions in which researchers from various perspectives are making efforts to develop systematic optimization tools to improve the performance of chemical reactors. The contributions reflect on the increasing awareness that textbook knowledge and heuristics (Levenspiel, 1962), commonly employed in the development of chemical

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reactors, are now deemed responsible for the lack of innovation, quality, and efficiency that characterizes many industrial designs.

From an economic viewpoint, final-product of the required quality demands a certain respectable maximal productivity of a chemical reactor. The reactor productivity depends on reaction rate, which usually increases exponentially with rising temperature.



Figure 1: Batch reactor with single external cooling jacket

DESCRIPTION OF A REACTOR

This work uses a mathematical model of a reactor shown in Figureure. 2. From constructional standpoint, the acts about the vessel with double side for cooling medium and is further equipped with stirrer for mixing reactionary mixtures.



Figure 2: Batch reactor

Reactor disposes by two physical inputs. First input denoted "Input Chemical *FK*" is chemical dosing into reaction about mass flow rate \dot{m}_{FK} , temperature T_{FK} and specific heat c_{FK} . Second input denoted "Input cooling medium" is water drain into the reactor double side with mass flow rate \dot{m}_V , temperature T_{VP} and specific heat c_V . This coolant further traverses among jacketed through space of reaction and his total weight in this space is m_{VR} . Coolant after it gets off the exit reaction denoted "output cooling medium" about mass flow rate \dot{m}_V , temperature T_V . At the beginning of the process there is an initial batch

inside the reactor with parameter mass m_P . Reactionary mixture then has total mass m, temperature T, specific heat c_R and stirs till the time chemicals FK described by parameter concentration a_{FK} .

Non-linear model of reactor

 $\dot{m}_{FV} = m'[t]$

Description of the reactor applies a system of four balance equations (1). The first one expresses a mass balance of reaction mixture inside the reactor, the second a mass balance of the chemical FK, and the last two formulate entalpic balances, namely balances of reaction mixture and cooling medium. Equations (1), where for simplified notation of basic equations (2) is represented by term "k".

$$\dot{m}_{FK} = m[t]a'_{FK}[t] + km[t]a_{FK}[t]$$

$$\dot{m}_{FK}c_{FK}T_{FK} + \Delta H_r km[t]a_{FK}[t] =$$

$$= KS(T[t] - T_V[t]) + m[t]c_R T'[t]$$
(1)
$$\dot{m}_V c_V T_{VP} + KS(T[t] - T_V[t])$$

$$= \dot{m}_V c_V T_V[t] + m_{VR} c_V T_V'[t]$$

$$k = Ae^{\frac{E}{RT[t]}}$$
(2)

After modification into the standard form, the balance equations are obtained in form (3)

$$m'[t] = \dot{m}_{FK}$$

$$a'_{FK}[t] = \frac{\dot{m}_{FK}}{m[t]} - Ae^{-\frac{E}{RT[t]}} a_{FK}[t]$$

$$T'[t] = \frac{\dot{m}_{FK}c_{FK}T_{FK}}{m[t]c_R}$$

$$+ \frac{Ae^{-\frac{E}{RT[t]}}\Delta H_r a_A[t]}{c_R} - \frac{KST[t]}{m[t]c_R} + \frac{KST_V[t]}{m[t]c_R}$$

$$T'_V[t] = \frac{\dot{m}_V T_{VP}}{m_{VR}} + \frac{KST[t]}{m_{VR}c_V} - \frac{KST_V[t]}{m_{VR}c_V} - \frac{\dot{m}_V T_V[t]}{m_{VR}}$$
(3)

The design of the reactor was based on standard chemical-technological methods and gives a proposal of reactor physical dimensions and parameters of chemical substances. These values are called in this participation expert parameters. The objective of this part of the work is to perform a simulation and optimization of the given reactor. Therefore into system equations (3) were instated constants:

 $A = 219,588 \text{ s}^{-1}, E = 29967,5087 \text{ J.mol}^{-1}, R = 8,314 \text{ J.}$ J.mol⁻¹.K⁻¹, c_{FK} = 4400 J.kg. K⁻¹, c_V = 4118 J.kg. K⁻¹, c_R = 4500 J.kg. K⁻¹, Δ Hr = 1392350 J.kg⁻¹,

K = 200 kg.s-3.K-1,

Next parameters, that are important for calculations are:

- Geometric dimension of the reaction: r[m], h[m]
- Density of chemicals: $\rho_P = 1203 \text{ kg.m-3}$,

 $\rho FK = 1050 \text{ kg.m-3}$.

• Stoicheiometric rate chemical:

$$m_P = 2,82236.m_{FK}$$

OPTIMIZATION OF PROCESS PARAMETERS AND THE REACTOR GEOMETRY

We illustrate the design approach using the batch reaction system shown in Figure. 1. The main aim in this example is finding the optimization of process parameters and the reactor geometry. Here, it is a optimization of batching value \dot{m}_{FK} together with process parameters of the cooling medium and including also reactor geometry and cooling area.

Mathematical problems

In this optimization was founded optimized parameters with one another linked ,so that heat transfer surface, volume, and hence also mass mixtures of reaction was mutually in relation. Heat transfer surface S have relation:

$$S = 2\pi r h + \pi r^2 \tag{4}$$

Where r is radius and h is high of the space reactor (see Figure.2)

Volume of vessel of rector applies to relation:

$$V = \pi r^2 h \tag{5}$$

Total mass of mixtures in the reaction is initial batch inside the reactor with parameter mass m_P a mass input chemical *FK* m_{FK} , that:

$$m = m_p + m_{FK} \tag{6}$$

The stechiometric ratio is given by (7).

$$m_P = 2,82236m_{FK} \tag{7}$$

Total volume of mixtures in the reaction equal sum of volume initial mixtures in the reaction and volume of FK:

$$V = V_{p} + V_{FK} = \frac{m_{p}}{\rho_{p}} + \frac{m_{FK}}{\rho_{FK}}$$
(8)

The relationship between the optimized volume of reactor and the mass of added chemical FK is given by (8). Then substituting to (7) gives the mass of the initial batch in the reactor.

$$m_{FK} = \frac{\rho_p \rho_{FK} V}{2,82236\rho_{FK} + \rho_p} \tag{9}$$

In this example, the optimization was then added parameter thickness d of vessel, which have relation that:

$$m_{VR} = \rho_V S d \tag{10}$$

In this optimization the point was to minimize the area arising as a difference between the required and real temperature profile of the reaction mixture in a selected time interval, which was the duration of a batch cycle. The required temperature was 97°C (370.15 K). The cost function (CF) that was minimized is given in (11):

$$f_{\cos t} = \sum_{t=0}^{t} \left| w - T[t] \right| \tag{11}$$

The CF has been calculated in general from the distance between desired state and actual system output.

Static optimization of reactor

The above described reactor, in the original set-up, gives unsatisfactory results. To improve reactor behavior, static optimization was performed using the algorithms SOMA and DE. In this work the optimization was performed by the following optimization of batching value reactor's parameters geometry.

Used Algorithm and Parameter Setting

For the experiments described here, stochastic optimisation algorithms, such as Differential Evolution (DE) (Price, 1999) and Self-Organizing Migrating Algorithm (SOMA) (Zelinka, 2004), had been used. Alternative algorithms, like Genetic Algorithms (GA) and Simulated Annealing (SA), are now in process, and results are hoped to be presented soon. Main reason why DE and SOMA has been sed comes from contemporary state in chemical engineering and EAs use. Since now has been done some research with attention on use of EAs in chemical engineering optimization, including DE. This participation has to show that applicability of relatively new algorithms ia also possitive and can lead to applicable results, as was shown for example in Zelinka (2001), which has been done under 5th EU project RESTORM (acronym of Radically Environmentally Sustainable Tannerv Operation by Resource Management) and main aim was to use EAs in chemical engineering processes. True is also that there is a plenty of other heuristic like particle swarm (Liu, Liu, Cartres, 2007), scatter search (Glover, Laguna, Martí, 2003), memetic algorithms, simulated annealing (Kirkpatrick, Gelatt, Vecchi, 1983), etc. and according to No Free Lunch teorem (Wolpert, Macready, 1997) is clear that each heuristic would be less or more applicable on example presented here. DE and SOMA has been also used because authors have satisfactorial experiencies with both algorithms. Very brief description is as follows.

Differential Evolution (Price, 1999) is a populationbased optimization method that works on real-number coded individuals. For each individual xi,G in the current generation G, DE generates a new trial individual x'i,G by adding the weighted difference between two randomly selected individuals xr1,G and xr2,G to a third randomly selected individual xr3,G. The resulting individual x'i,G is crossed-over with the original individual xi,G. The fitness of the resulting individual, referred to as perturbated vector ui,G+1, is then compared with the fitness of xi,G. If the fitness of ui,G+1 is greater than the fitness of xi,G, xi,G is replaced with ui,G+1, otherwise xi,G remains in the population as xi,G+1. Deferential Evolution is robust, fast, and effective with global optimization ability. It does not require that the objective function is differentiable, and it works with noisy, epistatic and time-dependent objective functions. Pseudocode of DE is:

1. Input :
$$D, G_{\max}, NP \ge 4, F \in \{0, 1+\}, CR \in [0, 1], \text{ and initial bounds } : \vec{x}^{(w)}, \vec{x}^{(h)}.$$

2. Initialize :
$$\begin{cases} \forall i \le NP \land \forall j \le D : x_{i,j, G=0} = x_j^{(h)} + rand_j [0, 1] \bullet (x_j^{(h)} - x_j^{(h)}) \\ i = \{1, 2, ..., NP\}, j = \{1, 2, ..., D\}, G = 0, rand_j [0, 1] \in [0, 1] \end{cases}$$
3. While $G < G_{\max}$
4. Mutate and recombine :
4.1 $r_i, r_2, r_3 \in \{1, 2, ..., NP\}, \text{ randomly selected, except } : r_i \neq r_2 \neq r_3 \neq i$
4.3 $\forall j \le D, u_{j,i,G+1} = \begin{cases} x_{j,n,G} + F \cdot (x_{j,n,G} - x_{j,r_2,G}) \\ i f (rand_j [0, 1] < CR \lor j = j_{rand}) \\ x_{j,i,G} \text{ otherwise} \end{cases}$
5. Select
 $\vec{x}_{i,G+1} = \begin{cases} \vec{u}_{i,G+1} & \text{if } f(\vec{u}_{i,G+1}) \le f(\vec{x}_{i,G}) \\ \vec{x}_{i,G} & \text{otherwise} \end{cases}$

SOMA is a stochastic optimization algorithm that is modelled on the social behaviour of co-operating individuals (Zelinka, 2004). It was chosen because it has been proved that the algorithm has the ability to converge towards the global optimum (Zelinka, 2004). SOMA works on a population of candidate solutions in loops called migration loops. The population is initialized randomly distributed over the search space at the beginning of the search. In each loop, the population is evaluated and the solution with the highest fitness becomes the leader L. Apart from the leader, in one migration loop, all individuals will traverse the input space in the direction of the leader. Mutation, the random perturbation of individuals, is an important operation for evolutionary strategies (ES). It ensures the diversity amongst the individuals and it also provides the means to restore lost information in a population. Mutation is different in SOMA compared with other ES strategies. SOMA uses a parameter called PRT to achieve perturbation. This parameter has the same effect for SOMA as mutation has for GA. The PRT Vector defines the final movement of an active individual in search space.

The randomly generated binary perturbation vector controls the allowed dimensions for an individual. If an element of the perturbation vector is set to zero, then the individual is not allowed to change its position in the corresponding dimension. An individual will travel a certain distance (called the path length) towards the leader in n steps of defined length. If the path length is chosen to be greater than one, then the individual will overshoot the leader. This path is perturbed randomly. For an exact description of use of the algorithms see (Price, 1999) for DE and (Zelinka, 2004) for SOMA. Pseudocode of SOMA is:

Input: $N, MigrationsPopSize \ge 2, PRT \in [0,1], Step \in (0,1], MinDive (0,1],$ PathLengthe (0,5], Specimenwith uper and lower bound $\mathbf{x}_{i}^{(h)}, \mathbf{x}_{i}^{(lo)}$

$$\begin{array}{l} \text{Inicialization} \\ \begin{cases} \forall i \leq PopSize \land \forall j \leq N : x_{i,j,Migration = 0} = x_j^{(lo)} + rand_j \begin{bmatrix} 0,1 \end{bmatrix} \bullet \begin{pmatrix} x_j^{(hi)} - x_j^{(lo)} \end{pmatrix} \\ i = \{1,2,...,Migration\$, \ j = \{1,2,...,N\}, \ Migration\$=0, \ rand_j \begin{bmatrix} 0,1 \end{bmatrix} \in \begin{bmatrix} 0,1 \end{bmatrix} \end{cases}$$

While *M*igrations<*Migrations*

 $\forall i \leq PopSize \begin{cases} While t \leq PathLength \\ if rnd_{j} < PRT pak PRTVector_{j} = 1 else0, \quad j = 1,...,N \\ x_{i,j}^{ML+1} = x_{i,j,start}^{ML} + (x_{L,j}^{ML} - x_{i,j,start}^{ML}) t PRTVector_{j} \\ f(x_{i,j}^{ML+1}) = \text{ if } f(x_{i,j}^{ML}) \leq f(x_{i,j,start}^{ML}) \text{ else } f(x_{i,j,start}^{ML}) \\ t = t + Step \\ Migrations= Migrations+1 \end{cases}$

The control parameter settings have been found empirically and are given in Tab. 1 (SOMA) and Tab. 2 (DE). The main criterion for this setting was to keep the same setting of parameters as much as possible and of course the same number of cost function evaluations as well as population size (parameter PopSize for SOMA, NP for DE). Individual length represents number of optimized parameters, see Tab. 3.

Table 1: SOMA parameter setting		
	А	
PathLength	3	
Step	0.41	
PRT	0.1	
PopSize	20	
Migrations	50	
MinDiv -1		
Individual Length	6	
CF Evaluations	6951	
Table 2: DE parameter setting		
^	A	
NP	20	
F	0.9	

NP	20
F	0.9
CR	0.2
Generations	200
Individual Length	6
CF Evaluations	4000

EXPERIMENTAL RESULTS

Due to the fact that EAs are partly of stochastic nature, a large set of simulations has to be done in order to get data for statistical data processing. Both algorithms (SOMA, DE) have been applied 100 times in order to find the optimum of process parameters and the reactor geometry. All important data has been visualized directly or/and processed for graphs demonstrating performance of both algorithms. Estimated parameters and their diversity (minimum, maximum and average) are depicted in Figure. 3 -Figure. 6 . From those pictures it is visible that results from both algorithms are comparable. For the demonstration are graphically the best solutions shown in Figure. 8, 10 and Figure. 12. There is shown time dependence of a_{FK} and T from both algorithms. The best values of parameter setting are recorded in Tab.3 & Tab. 4. On Figure. 7 - Figure. 22 are for example shown records of all 100 simulations and the best solutions of all 100 simulations (Fig. 7-14 for DE and Figure. 15-22 for SOMA).

The simulation results are sometimes different due to observed parameter since it depends on the number of migration loops. Futhermore, global minimum process function is corresponding to the oxies "z" of cost function, but it is the difference between the required state (stabilized fixed point) and the real system output on the whole simulation interval t.

 Table 3: Optimized reactor parameters and their range inside which has been optimization done

Parameter	Range
\dot{m}_{FK} [kg.s-1]	0-500
r [m]	0.3 - 3.0
h [m]	0.5 - 3.5
T_{VP} [K]	273.15 - 323.15
\dot{m}_V [kg.s-1]	0-10
d [m]	0.03 - 0.1

Table 4: The best values of optimized parameters by SOMA and DE

Parameter	SOMA	DE
\dot{m}_{FK} [kg.s-1]	0.00545104 0.04204	
r [m]	0.322817	0.543594
h [m]	0.50696	1.86628
T_{VP} [K]	315.873	294.718
\dot{m}_V [kg.s-1]	7.94792	9.94168
d [m]	0.0848451	0.0563635

Parameter diversity for repeated simulations

Results visualised on Figure. 7 - 22 are also numerically recorded in Tab. 5 for DE and Tab. 6 for SOMA.

Table 5: Estimated parameters for DE

Parameter	Min	Avg	Max
\dot{m}_{FK} [kg.s-1]	0.020 0.154		0.460
r [m]	0.318	1.754	2.996
h [m]	0.512	1.740	3.492
T_{VP} [K]	293.219	304.565	322.652
\dot{m}_V [kg.s-1]	2.349	9.227	9.997
d [m]	0.0300	0.0410	0.0834

Tab.6: Estimated parameters for SOMA

Parameter	Min	Avg	Max
\dot{m}_{FK} [kg.s-1]	0.005	0.025	0.077
r [m]	0.300	0.580	2.069
h [m]	0.500	1.583	3.415
T_{VP} [K]	293.326	307.351	322.321
\dot{m}_V [kg.s-1]	4.00591	8.386	9.998
d [m]	0.0300	0.0546	0.0968





Figure 8: The best solution for m (DE)











Figure 15: 100 simulations for m (SOMA)



Figure 16: The best solution for m (SOMA)



Figure 17: 100 simulations for aFK (SOMA)



Figure 18: The best solution for aFK (SOMA)



Figure 19: 100 simulations for T (SOMA)



Figure 20: The best solution for T (SOMA)







CONCLUSION

This paper has presented a systematic procedure to derive a solution model for operation of a dynamic chemical reactor process. The results produced by the optimizations depend not only on the problem being solved but also on the way how to define a given function.

The differences between both methods SOMA and DE are best seen in Tab.3 and tab.4. The first part shows the parameters of batch reactor designed by an expert, and the second part shows the parameters obtained through static optimization.

Calculation was 100 times repeated and the best, worst and average result (individual) was recorded from the last population in each simulation. All one hundred triplets (best, worst, average) were used to create Figure. 3 to Figure.6.

Both algorithms (SOMA, DE) have been applied 100 times in order to find the optimum of process parameters and the reactor geometry. The primary aim of this comparative study is not to show which algorithm is better or worse, but to show from the outputs of all simulations are depicted in Figure. 7-22 show that evolution SOMA represents the best solution from actual simulation more than DE. Based on data from all simulations, two comparison can be done. From parameter variation of view, the estimated parameters depicted in Figure.3–Fig.6 show that both algorithms are comparable in performance (with small deviations).

From the graphs, it is evident that the courses of SOMA algorithm are more densities in a thin specter and not far from the start of mass axis. Only few values drifting out of the specter. The results of the DE algorithm are speedier in the weight specter. From these results we may conclude, that SOMA has much better convergence then DE algorithm (see Figure.7 & Figure.15).

Basic optimizations presented here were based on a relatively simple functional. Unless the experimenter is limited by technical issues when searching for optimal geometry parameters, there is no problem in defining more complex functional including as subcriteria e.g., stability, costs, time-optimal criteria, controllability, etc. or their arbitrary combinations.

Finally, on the basis of presented results, it may be stated that the reactor parameters have been found by optimization which demonstrates performance superior to that of reactor set up by an expert. Future work objective is to formalize this process in order support the control system design to the best extent possible. According to all results obtained during time it is planned, the main activities would be focused expanding of this comparative study for genetic algorithms and simulated annealing. Furthermore, for the successful stabilization is to analyse more cost function CF.

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SOLVING A MULTI-DIMENSIONAL KNAPSACK PROBLEM USING A HYBRID PARTICLE SWARM OPTIMIZATION ALGORITHM

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KEYWORDS

Particle Swarm Optimization, Multi-Dimensional Knapsack Problem

ABSTRACT

In this paper, an optimisation technique based on the Particle Swarm Optimization (PSO) algorithm will be experimented upon the Multi-dimensional Knapsack Problem. Through the merging of fundamental concepts of the existing PSO algorithm and selected features of evolutionary algorithms, a novel hybrid algorithm is created. When testing the algorithm against a test suite publicly available on OR-LIB, it was discovered that the algorithm is able to locate fitness values very close to best available results discovered using Linear Programming techniques, even though the algorithm is at the very early stage of development. Such an observation reveals the potential of this algorithm, calling for further research to be made upon it.

INTRODUCTION

The knapsack problem is an NP hard problem, and is part of a family of combinatorial problems (Martello and Toth, 1990). In the knapsack problem, the process of packing items with cost and profit associated to them into a container is simulated. Typically, the aim is to maximise the fitness, at the same time not exceeding supplied constraints. Given its simplicity, it can be used to test the performance of an algorithm in a discreet search space, and can act as a model for practical applications such as financial portfolio optimization and engineering design optimization.

Amidst the many different types of knapsack problems is the Multi-dimensional Knapsack Problem (MKP), which extends upon the basic knapsack problem with an additional dimension (Chu and Beasley, 1998). Instead of having just one constraint, the number of constraints can increase, which makes it possible to simulate a larger range of real-world optimization problem. The MKP can be described mathematically as follow: maximise

$$f = \sum_{i=1}^{n} f_i \cdot \delta_i \tag{1}$$

given equations

$$B_j \ge \sum_{i=1}^n u_{ij} \cdot \delta_i \tag{2}$$

$$\delta_i \in \{0, 1\}, \quad i = 1, ...n, \quad j = 1, ...m$$
 (3)

Legend

 $\overline{i = \text{identifier of candidate items}}$

n = number of candidate items

j = identifier of constraints

m = number of constraints

f =fitness value

 $u_{ij} = \text{cost value of item } i, \text{ constraint } j$

 B_i = maximum cost value of constraint *j*

 $\delta_i = 0/1$ value determining if the item *i* is in the knapsack

LITERATURE SURVEY

In this section, a detailed review on existing literature will be presented in a systematic manner. Existing attempts that tackle the MKP is initially presented, followed by fundamental concepts of the original Particle Swarm Optimization (PSO) algorithm.

Previous Attempts on the MKP

A quick survey on existing literature reveals that a range of well known stochastic algorithms have been tested on the MKP. In their paper, Chu and Beasley (1998) attempted to solve the MKP using Genetic Algorithms, and obtained good results using less computational effort as opposed to many other techniques which include the CPLEX MIP solver. While the results are not as good as those obtained using Linear Programming techniques, which serve as the benchmark in their test, it demonstrates that a stochastic algorithm is able to locate results that are very close to the known optimum under less time, and is useful for applications where the efficiency of an algorithm is a decisive factor. This success led other researchers to test difference stochastic algorithms

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) against the MKP, for example, Qian and Ding (2007), who tested the Simulated Annealing algorithm against the Chu and Beasley test suite and Hembecker et.al. (2007), who tested the PSO algorithm against smaller instances of the same test suite. While it was reported in both work that Simulated Annealing and PSO are unable to locate results as good as the one located using Genetic Algorithm, the test results are still valuable as it give researchers an indication of heuristics that are less suitable in solving the MKP, and provide inspiration to create a hybrid algorithm that contains the strengths of different algorithms.

The Original PSO Algorithm

PSO is fundamentally a stochastic, population-based search algorithm which mimics organisms that interact as a swarm such as a school of fish or a swarm of bees looking for food. Its creators (Kennedy and Eberhart, 1995) found elegance in design by observing the social interaction and learning behaviour of swarm-based animals; the animals do not travel randomly in search for food but have an observable pattern, where information such as the nearest 'patch' of food is shared among individuals in the swarm.

With the above heuristic in mind, Kennedy and Eberhart later created a mathematical formula to mimic the behaviour above, as seen in notations (4) and (5).

$$v_{a,b} \leftarrow c_1 r_1(gbest_b - x_{a,b})$$

$$+ c_2 r_2(pbest_{a,b} - x_{a,b})$$
(4)

$$x_{a,b} \leftarrow x_{a,b} + v_{a,b} \tag{5}$$

Legend

 $v_{a,b} = Velocity of ath Particle in bth Dimension$ $<math>x_{a,b} = Position of ath Particle in bth Dimension$ $<math>c_1, c_2 = Constant parameters controlling influence$ $<math>r_1, r_2 = Random number$ $gbest_b = Position of global best particle$ $<math>pbest_{a,b} = Position of particle's previous best position$

To implement the PSO algorithm in a computing environment, the algorithm's particles, or agents, are encoded to represent candidate solutions in an n-dimension search space. Each agent has an associated velocity, which dictates how the agent travels in the search space. By calculating the position of an agent based on its velocity, new candidate solutions in each iteration or measured timeframe can be obtained. Also, each agent will have knowledge of its previous best fitness and the global best fitness of the swarm. This knowledge will be used to influence the velocity of the agents, and can be seen in mathematical notation (4). With constant parameters that control global influence and local influence, it allows the user to have the flexibility in controlling the algorithm's behaviour. On the other hand, random numbers reduce the chances of premature convergence by introducing the element of randomness. Using the above heuristic, the velocity of the agents will be calculated, and the agents will move according to a certain velocity using the formula illustrated in notation (5). This will be repeated until a stopping condition is met.

By studying the above algorithm, it can be seen that the original PSO is intended for problems which are contiguous in nature. In 1997, Kennedy and Eberhart proposed a customised version of their PSO algorithm to tackle problems in a discrete search space. In this version, the trajectories of agents are calculated from the probability of whether the next coordinate will be either one or zero. Instead of using notation (5) to update the velocity and position of the particles, the sigmoid function in (6) is used, and (7) calculates the trajectory in the binary search space.

$$s(v_{a,b}) = \frac{1}{(1 + \exp(-v_{a,b}))}$$
(6)

if
$$r < s(v_{a,b})$$
 then $x_{a,b} = 1$; else $x_{a,b} = 0$ (7)

$\frac{\text{Legend}}{r = \text{Random number}}$

While the original discrete PSO is successful in many cases, it is interesting to see if it can be simplified by replacing some of its operators with those found in evolutionary algorithms while still maintaining the behaviour demonstrated by PSO. One of the reasons why this is being looked into is because the probability of a bit being 1 or 0 is calculated and later assigned to every bit in all agents of the swarm, and this operation may be computationally expensive. Wang (2007) approached this problem by replacing (6) and (7) with operations based on Estimation of Distribution - a technique which generates new solutions using probabilistic models of the distribution of regions, and have shown that in their test cases is superior compared to the algorithm proposed by Kennedy and Eberhart (1997). In the paper, the simplification process will be taken further, where a Hybrid PSO algorithm that is partly inspired by the use of inheritance operators in Tseng and Liao (2008) will be proposed in the next section.

PROPOSED IDEAS

In this section, a number of new customisations of the PSO algorithm are proposed. By using these new and novel concepts, search algorithms that have the strengths of different algorithms in this area of research are created.

A Hybrid PSO Algorithm

In this paper, an operator in evolutionary algorithm called inheritance, which is illustrated in Figure 1, will be adapted for the PSO algorithm to replace the position updating operation based on velocity and probability. Such a technique relies on the idea that the more similar two agents are, the closer they are to each other.

Essentially, it is proposed that a controlled number of bits are selected randomly from the parent agent, and applied to the corresponding position of the child agent. This mechanism can be applied onto the heuristics where information from the global best agent (gbest) and information from previous memory (pbest) needs to be transferred to a particular agent, which can be controlled by the bits to copy from gbest and bits to copy from pbest parameters respectively. This is possible as the one-way sharing mechanism allows information of a child to be inherited from multiple sources, in which a child can have multiple parents, making it not just limited to the parents mentioned above. Furthermore, with parameters that control the number of bits to inherit, it gives the user the ability to control the behaviour of the algorithm, thus allowing the flexibility of building highly dynamic and complex algorithms that rely on a large number of heuristics. Do note that as the parameter can be changed during runtime, it is possible to dynamically change the behaviour of an algorithm when it is executing, though this significantly complicates the parameter tuning process.

Besides the inheritance operator, it is also proposed that an adapted mutation operator is used to introduce the element of randomness into the algorithm, substituting the r_1 and r_2 variables in the formula proposed in notation (4). This mutation operator works by random flipping a bit of the search agent, where the chance of flipping is determined by a parameter called mutation rate. One of the key benefits of the mutation operator proposed as opposed to the random variables r_1 and r_2 of the original PSO is the degree of randomness that can be introduced is controllable in a separate manner. In order to encourage exploration, a high mutation rate value can be set. Setting a low value reduces the stochastic factor, and allows other heuristics to affect the algorithm to a higher extent. It needs to be noted that this is different from the v_{max} parameter used by Kennedy and Eberhart (1997), as the v_{max} parameter controls the distance an agent can ultimately travel, whereas the proposed parameter controlling the degree of mutation does not directly affect the inheritance operation.

Repair Operation

By using the algorithm above, it is possible that an agent can contain a solution that does not conform to its constraints. In order to overcome this problem, a random bit that contains the value 1 is switch to the value 0, and a fitness evaluation is then performed to ensure the value is within its constraints. This is then repeated until the solution satisfies all constraints, and the entire operation resembles the action of taking out items from the knapsack until the no constraints are violated. As this operation is considered a significant part in locating a solution, it is decided that every repair operation performed is measured and included in the results related to the efficiency aspect of the algorithm.

EXPERIMENT FRAMEWORK

The purpose of this section is to document the steps involved in the implementation and testing of the ideas proposed in previous chapters. Reproducibility of the experiments is of primary concern due to the stochastic nature of the algorithms tested.

The OR-LIB Test Suite

For comparison and analysis purposes, the MKP test suite published on OR-LIB by Chu and Beasley (1998) is being used for testing the performance of the algorithm proposed earlier. There are a number of reasons why this approach was chosen. Firstly, using a publicly accessible test suite makes it possible for the reader to compare presented results against other results published in other literature. Doing so allows the strengths and weaknesses of the proposed algorithm to be identified, facilitating the decision making process when choosing a suitable algorithm. Secondly, such an approach also facilitates the reproduction of the experiment compared to approaches where the test data is generated dynamically. One of the concerns of using dynamically generated test data is that the tested algorithm may behave differently, due to the difference in test data. Having a consistent benchmark removes this concern, allowing the tested algorithms to be compared more fairly.

Measurement Approach

In order to evaluate the effectiveness of the algorithm, the best known fitness values, which are obtained using Linear Programming (LP) techniques and included in the test suite, are used as a benchmark. Using the formula in (8), the gap between the best known results and the results presented can be obtained. As the derived value is a percentage value, having a smaller value indicates that the obtained result is closer to the best known result, in which having a gap value of 0% means the algorithm succeed in obtaining the best known result.

$$\frac{f_{bestknown} - f_{obtained}}{f_{bestknown}} \times 100 \tag{8}$$

With regard to the efficiency aspect of the algorithm, the number of total fitness evaluations performed in order to achieve the best obtainable value is used as a measurement. The diligent reader might notice that this approach is different compared to the approach used in other literature, where efficiency is usually measured in terms of execution time. There are a number of reasons why this approach is not chosen. Firstly, the environment in which



 $\overline{X} = Value not changed$

Figure 1: Parameter Controlled Position-Point Inheritance

the experiment is run on can significantly affect its execution time. There are differences in hardware such as CPU speed, CPU types and differences in software such as the Operating System used, influence of other programs in a multi-tasking systems, and programming platform that can skew the result. Because it is extremely difficult to recreate an environment that is exactly the same as the one it is run on, a measurement that is not affected by these factors is selected. While it can be argued that doing so makes it difficult to compare the efficiency of the algorithm against results published in existing literature, this can be overcame by recreating and testing candidate algorithms in the same environment.

Algorithm Parameters

Being a novel algorithm, parameters for the proposed algorithm need to be identified, and this is one of the challenges in getting the algorithm to work in an optimum manner. For this experiment, the parameters used are derived from the author's previous work, where the proposed algorithm was tested on a much smaller knapsack and a set of parameters is obtained using a simple parameter tuning process (Wan, 2008). Due to differences in the size of the knapsack (n), the parameters are scaled according to the size of the knapsack, and are listed in Table 1. With regard to the stopping condition, the experiments in this paper terminate once 15×10^6 fitness evaluations are made, which include fitness evaluations made during repair operations. While it can be argued that such a parameter tuning process does not guarantee the best set of parameters is obtained, it serves as a good starting point for setting up initial experiments. Once the proposed algorithm has been better understood, work should be conducted in this area to ensure that a set of parameters is readily available.

RESULTS AND DISCUSSION

The experiment results are presented in Table 2, and this is accompanied by test results obtained from work by Chu and Beasley (1998) and Qian and Ding (2007) for comparison purposes. By comparing the average of the Table 1: Parameters for Proposed Algorithm

Name	Value
Bits to copy from gbest	8% of <i>n</i>
Bits to copy from pbest	30% of <i>n</i>
Mutation Rate	0.33
Swarm Size	150% of <i>n</i>

average % gap values for each algorithm located at the bottom of the table, it can be seen that the proposed algorithm is able to locate results that are better than results from Qian and Ding, but is slightly less favourable as opposed to results from Chu and Beasley. While this may indicate that the Genetic Algorithm implemented by Chu and Beasley is able to perform better than the proposed algorithm for the MKP, the reader needs to bear in mind that this is an algorithm still in the early stage of development, and there is room to further improve the proposed algorithm. Firstly, it needs to be stressed that the parameter tuning process used is very simplistic, and it is possible that using a set of parameters obtained from a better parameter tuning process can yield better results. Secondly, the repair operator used by the proposed algorithm is based on a very simple heuristic, whereas the repair operator used in Chu and Beasley is complex and expensive in computational term, for example, the number of fitness evaluations needed. It is possible that the proposed algorithm can be improved by replacing the repair operator with the one proposed by Chu and Beasley. Finally, due to the simplicity and extensibility of the proposed algorithm, it is possible to invent new heuristics and append it to the proposed algorithm. A list such of heuristics exists, and is documented in previous work (Wan, 2008).

Key findings aside, analysis of the results obtained reveals that similar to results obtained by Chu and Beasley and Qian and Ding, the proposed algorithm has the highest average percentage gap for problems with small knapsack size, high number of constraints and small tightness ratio (m = 30, n = 100, $\alpha = 0.25$), indicating that this a set of test instances that are difficult to solve. With regard to the efficiency aspect of the algorithms, it is unfortunate that different approaches are used to measure the efficiency of a search, hence making a fair comparison between different algorithms very difficult. Nevertheless, it can be seen that for the proposed algorithm, the number of fitness evaluations required to locate the best solution increases as the size of the knapsack grows larger, and it is reasonable to believe that this applies to knapsacks with size larger than 500. Because the efficiency of an algorithm still plays a significant role when deciding if it is suitable for an application, future work that evaluates the efficiency of a range of algorithm is need, with great emphasis given to maintain a consistent execution environment that is able to provide accurate measurements.

CONCLUSION

Based on the key findings, it can be concluded that the proposed algorithm is able to locate a fitness value that is close to the best fitness values reported in the literature, which were obtained using linear programming. Seeing that this simple, extensible algorithm is still in the early stage of development, there exist the potential to increase its performance with better sets of parameters or addition of new heuristics. It is hoped that these finding will inspire future researchers in analysing the proposed algorithm from different perspectives to further improve upon it.

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	Proble	em	Chu and Beasley (1998)	Proposed Al	gorithm	Qian and Ding (2007)
т	п	α	Average % Gap	Average % Gap	AFEBS	Average % Gap
5	100	0.25	0.99	1.16	4,431,497	2.95
		0.50	0.45	0.53	3,848,719	1.67
		0.75	0.32	0.36	3,792,008	0.87
5	250	0.25	0.23	0.58	8,609,279	3.09
		0.50	0.12	0.25	10,281,679	1.89
		0.75	0.08	0.15	7,334,528	0.84
5	500	0.25	0.09	0.89	10,169,920	3.41
		0.50	0.04	0.33	10,306,961	2.04
		0.75	0.03	0.17	10,827,946	0.92
10	100	0.25	1.56	2.22	7,351,304	3.93
		0.50	0.79	1.01	4,615,686	2.09
		0.75	0.48	0.61	3,934,004	1.06
10	250	0.25	0.51	1.09	9,693,256	3.21
		0.50	0.25	0.47	9,203,460	2.14
		0.75	0.15	0.27	8,024,108	1.01
10	500	0.25	0.24	1.30	10,302,268	3.67
		0.50	0.11	0.56	11,252,190	2.50
		0.75	0.07	0.26	11,243,238	1.17
30	100	0.25	2.91	3.69	3,263,436	4.94
		0.50	1.34	1.62	4,621,375	2.62
		0.75	0.83	1.04	1,993,596	1.29
30	250	0.25	1.19	1.91	7,331,979	3.60
		0.50	0.53	0.77	8,692,707	2.25
		0.75	0.31	0.46	7,013,305	0.96
30	500	0.25	0.61	1.83	10,434,576	3.75
		0.50	0.26	0.75	10,706,743	2.30
		0.75	0.17	0.37	10,489,562	1.07
	A	verage	0.54	0.91	7,769,234	2.27

Table 2: Computational Results from Chu and Beasley (1998), Proposed Algorithm and Qian and Ding (2007)

AFEBS = Average number of Fitness Evaluations to obtain Best Solution

A NEW STOCHASTIC ALGORITHM FOR THE CAPACITY & FLOW ASSIGNMENT PROBLEM AND AN ASSOCIATED RATE OF CONVERGENCE

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Agents, learning, intelligent systems, optimization, operations research

ABSTRACT

In this paper we examine the problem of optimizing the average time latency of a network using agents that are able to learn. The network design is constrained by a traffic matrix which dedicates specific flows between specific pairs of nodes. Although this is an analysis of an application, we only present two methodologies here, i.e. an algorithm for optimization and a corresponding conservative rate of convergence based on no learning. The application part will be presented in the near future once data is available. We expect the tools developed in this paper can be used to optimize a wide range of objective functions. They will not be limited to optimizing time latency.

BACKGROUND

As part of a Technology Investment Fund project on network-centric warfare (Ng et al. 2006) currently being conducted at the Defence Research and Development Canada Centre for Operational Research and Analysis, we aim to optimize the time latency of a defence network. An example of such a network is the one implemented at Defence Research and Development Canada – Atlantic known as the Networked Underwater Warfare Technology Demonstration Program (LeFrançois 2004). The time latency of a network can be determined in many ways. However, in this paper we describe a methodology designed to optimize time latency using agents that have the ability to learn. The main results of this paper are to provide an algorithm to do so and to derive the rate of convergence of the corresponding algorithm when no learning is in effect. Our methodology draws on (Oommen and Roberts 2000), which provides a heuristic algorithm to optimize a cost objective function.

LEARNING ALGORITHM

We examine a communication network that has a global maximum capacity *C*. The network flows must satisfy the traffic matrix (γ_{uv}). That is, there will be a dedicated flow from node *u* to node *v* that is greater than or equal to γ_{uv} . This ensures that node *u* can communicate with node *v* with the desired flow γ_{uv} . In addition, the time latency of the network depends on both the flow and the capacity of each link. We make use of the algorithm in (Oommen and Roberts 2000) which is described below.

The capacities of the links are represented by a vector $(c_1, c_2, ..., c_e)$, where *e* is the number of edges or links in the network, and c_i is chosen from a finite set of capacities such as (0,1,2,...), where a capacity unit corresponds for example to 1200 *bps* (bits per second). For each link *i* and each possible capacity *j*, there is a triplet (I_{ij}, S_{ij}, D_{ij}) , where I_{ij} is the probability that the current capacity *j* of the link *i* should be increased, S_{ij} is the probability that the current capacity *j* of the link *i* should be increased, S_{ij} is the probability that the current capacity *j* of the link *i* should remain unchanged, and D_{ij} is the probability that the current capacity *j* of the link *i* should be decreased. The capacity *j* of a link *i* is modelled as an agent whose

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learning process is encoded in the evolution of the triplet (I_{ij}, S_{ij}, D_{ij}) .

The final solution vector will consist of the capacities c_i such that S_{ij} probability values approach unity, e.g. 0.99. The closer this value is to unity, the more accurate is the solution. As is often the case with heuristic algorithms, (Oommen and Roberts 2000) did not provide the rate of convergence of their algorithm. Fortunately, it is possible to derive the rate of convergence for this algorithm at least in the case where agents do not learn. But before we present the derivation for the rate of convergence, we show below the pseudo code in (Oommen and Roberts 2000). The algorithm can be divided into three modules. Module 1 initializes the triplet (I_{ii}, S_{ii}, D_{ii}) , looks for a feasible solution and determines its value as dictated by the objective function. Module 2 searches the solution space. Module 3 updates the triplet (I_{ij}, S_{ij}, D_{ij}) .

The remainder of the section and the example below illustrate the pseudo code and are taken almost verbatim from (Oommen and Roberts 2000).

Example. Let us assume that the capacity j of a link i has been lowered, such that $j \leftarrow j-1$, resulting in a lower cost feasible solution. This means that we take the following steps.

1. Since the solution vector is feasible, we shall raise the decrease probability D_{ii} , as:

$$\begin{split} I_{ij}\left(t+1\right) &= \lambda_{R1} \cdot I_{ij}\left(t\right) \\ S_{ij}\left(t+1\right) &= \lambda_{R1} \cdot S_{ij}\left(t\right) \\ D_{ij}\left(t+1\right) &= 1 - \left(I_{ij}\left(t\right) + S_{ij}\left(t\right)\right) \end{split}$$

In general,

- a. If the capacity was increased, raise D_{ij} .
- b. If the capacity stayed the same, raise S_{ii} .
- c. If the capacity was decreased, raise D_{ii} .

2. Now, since the solution vector results in a lower network cost, the stay probability S_{ij} should be raised. This is done as follows:

$$I_{ij}(t+1) = \lambda_{R2} \cdot I_{ij}(t)$$
$$D_{ij}(t+1) = \lambda_{R2} \cdot D_{ij}(t)$$
$$S_{ij}(t+1) = 1 - (I_{ij}(t) + D_{ij}(t))$$

In general,

- a. If the capacity was increased, raise D_{ij} .
- b. If the capacity stayed the same, raise S_{ij} .
- c. If the capacity was decreased, raise S_{ii} .

Similar steps are performed for each of the possible scenarios that are examined during the execution of the algorithm. This process continues until all the link capacities c_i have S_{ij} probability values that are close enough to unity.

Module 1. Initialize the triplet (I_{ii}, S_{ii}, D_{ii}) .

For (i = 1 to maxlinks(=e))

For (j=1 to maxcaps(=C))

If (j = 1 (left-boundary-state))

 $I_{ij} = 1, S_{ij} = 0, D_{ij} = 0$

End-If

If $(j = \max caps (right-boundary-state))$

$$I_{ij} = 0$$
, $S_{ij} = 0$, $D_{ij} = 1$

End-If

If (1 < j < C (internal-state))

$$I_{ij} = 1/3$$
, $S_{ij} = 1/3$, $D_{ij} = 1/3$

End-If End-For End-For

Repeat

For (*i* =1 to maxlinks)

 $c_i = RAND(0, maxcaps)$

End-For

Until (network is feasible)

current-objective = calculate-objective()

For (i = 1 to maxlinks)

 $best - c_i = c_i$

End-For

best-objective = current-objective()

Module 2. Search the solution space.

While (count<num-iterations) and (accuracy-level (all links) < required accuracy)

For (i = 1 to maxlinks)

 $Action_i = RAND(Increase_{ii}, Stay_{ii}, Decrease_{ii})$

If $(Action_i = Increase_{ii})$

 $c_i = c_i + 1$

End-If

If $(Action_i = Decrease_{ii})$

 $c_i = c_i - 1$

End-If

current-objective = calculate-objective()

End-For

For (i = 1 to maxlinks)

 $j = c_i$

If (network is feasible)

If ($Action_i = Increase_{ii}$)

$$Raise(D_{ij}, \lambda_{R1})$$

End-If

$$\mathbf{If}\left(Action_{i} = Stay_{ij}\right)$$

 $Raise(S_{ij}, \lambda_{R1})$

End-If

If $(Action_i = Decrease_{ii})$

 $Raise(D_{ij}, \lambda_{R1})$

End-If

Else

Reset all links to best-objective capacities

End-If

If (network is feasible) and (current-objective < best-objective)

If (
$$Action_i = Increase_{ij}$$
)

Raise
$$(D_{ii}, \lambda_{R2})$$

End-If

If ($Action_i = Stay_{ij}$)

Raise $\left(S_{ij}, \lambda_{R2}\right)$

End-If

If
$$(Action_i = Decrease_{ii})$$

Raise
$$\left(S_{ij}, \lambda_{R2}\right)$$

End-If

For (i = 1 to maxlinks)

$$best - c_i = c_i$$

End-For

best-objective = current-objective()

End-If

End-For

End-While

Module 3. Procedure **Raise** – Updating the triplet (I_{ij}, S_{ij}, D_{ij}) . $\lambda_R = \lambda_{R1}$ is associated with a new feasible solution. $\lambda_R = \lambda_{R2}$ is associated with a new feasible solution that is also superior.

If (Action = Increase) $D_{ij} = \lambda_R \cdot D_{ij}$; $S_{ij} = \lambda_R \cdot S_{ij}$; $I_{ij} = 1 - (D_{ij} + S_{ij})$

End-If

If (Action = Stay)

$$I_{ij} = \lambda_R \cdot I_{ij}; \ D_{ij} = \lambda_R \cdot D_{ij}; \ S_{ij} = 1 - (I_{ij} + D_{ij})$$

End-If

If (Action = Decrease) $I_{ij} = \lambda_R \cdot I_{ij}$; $S_{ij} = \lambda_R \cdot S_{ij}$; $D_{ij} = 1 - (I_{ij} + S_{ij})$

End-If

ALGORITHM EXTENSION

We model the capacity assignment in the same way as that of (Oommen and Roberts 2000) (see above). Hence, there is a triplet $(I_{ij}^{(c)}, S_{ij}^{(c)}, D_{ij}^{(c)})$ associated with link *i* and capacity *j*, and the superscript *c* stands for capacity. In addition, we model in a similar way each path *l* as an agent that carries *k* units of flow and which connects node *u* to node *v*. Each path type agent is represented by a triplet $(I_{wvlk}^{(p)}, S_{wvlk}^{(p)}, D_{wvlk}^{(p)})$ where the superscript *p* stands for path. These triplets are updated at each run depending on random numbers and whether the objective function is improved or not. For example, if the objective function is improved then both $S_{ij}^{(c)}$

and $S_{uvlk}^{(p)}$ are increased. This new algorithm is the first main result of this paper and can be used to optimize the average time latency of a network, as defined in (Mostafa and Eid 2000):

$$T = \frac{1}{\sum_{uv} \gamma_{uv}} \cdot \sum_{k} \frac{f_k}{c_k - f_k} \tag{1}$$

where (u, v) represents node u and node v; each k represents a link while f_k and c_k are the flow and capacity of that link. We use enumeration to generate all possible paths that connect node u to node v. By modelling each path as an agent, we ensure flow conservation through each node. The flow through a link is then equal to the sum of the flows of all paths that traverse that link. For example, let $\{a, b, c, d, e\}$ be the set of nodes of a complete graph (all possible links) as shown on the LHS of Fig 1. Let's consider the link (a-b); path1 be (a-b-c) with 2 units of flow, path2 be (a-b-d) with 1 unit of flow and path3 be (c-a-b) with 3 units of flow. The flow through the link (a-b) will be the sum of 2+1+3 as each of the three paths traverse (a-b). Note that the flow of a link ranges from zero to C (the maximum capacity of the network).

RATE OF CONVERGENCE ASSUMING NO LEARNING



Fig 1 – An example of flows in a graph on the LHS and a defence network on the RHS.

We define the rate of convergence as the probability that a globally optimal state is found at least once as a function of number of iterations in a similar way to that in (Rajasekaran 1990). The rate of convergence that we derive below assumes no learning. Since the purpose of learning is to accelerate the convergence of the algorithm, we expect that this rate of convergence is a conservative estimate of the algorithm. We observe that for a link i, the flow through that link is regulated by a Markov chain as shown in Fig 2. Each flow state is labeled by a number. For example, the label 0 indicates that the flow is equal to zero (unit of flow), while the label 1 indicates that the flow is equal to one (unit of flow) etc. The connections between the labels show the transitions among the states.

The Markov chain shown in Fig 2 can be represented by a transition matrix P where P_{ij} is the probability that state *i* transitions into state *j*. For example, given C = 4, we get:



Fig 2 - A Markov chain.

$$P = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 \\ 0 & 1 & 0 & 0 & 0 \\ 2 & a & a & a & 0 & 0 \\ 0 & a & a & a & 0 & 0 \\ 0 & 0 & a & a & a & a \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$
(2)

where a = 1/3. We model *P* that way so that the states with flow equal to zero or *C* are not considered feasible. If a flow of a link is equal to zero then there is no communication necessary. Hence, the probability of transition from state zero to state one is set to 100 %. If a flow of a link is equal to *C* then there is no capacity left for the remaining links, which can happen only when we

have only one link in the network. However, the network that we consider consists of many links. Hence, the probability of transition from state C to state C-1 is also set to 100 %. Additionally, for j = 1, ..., C - 1, given link i, $P_{j,j-1}$ (the probability that state j transitions to state j-1) is equal to $D_{i,j} = a$; $P_{j,j}$ (the probability that state *j* stays the same) is equal to $S_{i,j} = a$; and $P_{j,j+1}$ (the probability that state j transitions to state j+1) is equal $I_{i,i} = a$. to For example, $P_{1,0} = P_{1,1} = P_{1,2} = a = D_{i,1} = S_{i,1} = I_{i,1}$ while all other transitions from state 1 are forbidden.

Lemma 1. The probability that the flow through a path is optimal is greater than or equal to:

$$p_f \ge 1 - \frac{C-2}{\left(C-1\right)^2} \cdot \left| \mathcal{Q}_f^n \right| \tag{3}$$

where *n* is the number of iterations; P_f is the transition matrix associated with the flow of a path; Q_f is equal to P_f with the exceptions that the first row, first column, last row and last column elements are set to zero; and $|Q_f^n|$ is the sum of all elements of Q_f^n . That is,

$$\left|\mathcal{Q}_{f}^{n}\right| = \sum_{i} \sum_{j} \left(\mathcal{Q}_{f}^{n}\right)_{i,j}$$

For example, given C = 4, we get:

$$Q_{f} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & a & a & 0 & 0 \\ 0 & a & a & a & 0 \\ 0 & 0 & a & a & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}; |Q_{f}| = 7 \cdot a (4)$$

Note that, P_f and Q_f do not change with n. This is so as there is no learning. However, when learning is in effect, the elements of P_f and Q_f are updated through the triplets (I, S, D).

Proof of Lemma 1. To alleviate the notation, we suppress the subscript f associated with P and Q. Let the optimal flow be f^* . We wish to determine the probability that a random and non-optimal flow i transitions to another also random and non-optimal flow j. The probability that we pick a random flow such that $i \neq f^*$ is:

$$P(flow = i \neq f^*) = (C-2)/(C-1)^2$$

For example, given C = 4, there are five possible states belonging to $\{0,1,2,3,4\}$. A random flow can be equal to any of these five states. However, if we discard state zero and state four as non-feasible states, there remain only three states. Hence the probability that we pick a random and feasible flow *i* is 1/(C-1) = 1/3. Further, if $f^* = 3$, then the probability that a random and feasible flow is not optimal (C-2)/(C-1) = 2/3. As a result, the probability that we pick a random flow *i* and that flow *i* is feasible and not optimal is $(C-2)/(C-1)^2 = (1/3) \cdot (2/3)$.

The probability that we start with a feasible flow $i \neq f^*$ and end up with another feasible flow $j \neq f^*$ is regulated by the transition matrix *P*. That is,

$$P(i \neq f^* \rightarrow j \neq f^*)$$

$$\leq P(i \neq f^*) \cdot P_{i,j} = (C-2)/(C-1)^2 \cdot P_{i,j}$$
(5)

The probability that we start with *any* feasible flow $i \neq f^*$ and end up with *any* other feasible flow $j \neq f^*$ is the sum of the above expression over *i* and *j* such that $i, j \neq f^*$, i.e.

$$(C-2)/(C-1)^2 \cdot \sum_{i,j \neq f^*} P_{ij}$$

We further observe that

$$\sum_{i,j\neq f^*} P_{i,j} \le \sum_{i,j} P_{i,j}$$

since all the elements of the transition matrix P are non-negative and the LHS sums over all elements i and j such that $i, j \neq f^*$, while the RHS sums over all elements i and j with no restrictions. That is, the sum on the RHS includes more elements of P than the sum on the LHS. Therefore,

$$(C-2)/(C-1)^2 \cdot \sum_{i,j \neq f^*} P_{i,j}$$

 $\leq (C-2)/(C-1)^2 \cdot \sum_{i,j \neq f^*} P_{i,j}$

Additionally, the sum on the RHS above runs over the states that are feasible and non-optimal, meaning that $i, j \neq 0, C$. This can be interpreted in a way such that the RHS above includes all transitions from a state *i* that is feasible to a state *j* that is also feasible. Therefore, all transitions from (to) 0 or *C* to (from) a feasible state are forbidden. This is equivalent to replacing P_{ij} with Q_{ij} . Repeating this argument *n* times, we get an upper bound for the probability q_f of not achieving the optimal state after *n* iterations:

$$q_{f} \leq (C-2)/(C-1)^{2} \cdot \sum_{i,j} Q_{i,j}^{n}$$
$$= (C-2)/(C-1)^{2} \cdot |Q^{n}|$$

Therefore, the lower bound to the probability $p_f = 1 - q_f$ of achieving the optimal state satisfies:

$$p_f \ge 1 - (C - 2) / (C - 1)^2 \cdot |Q^n|$$

Lemma 2. The probabilistic bound in Eqn (3) of finding the optimal flow is an increasing function of n.

Proof of Lemma 2. This is true as

$$Q^{n+1} = Q^n \cdot Q = Q^n \cdot (P - \Delta)$$

where $\Delta = P - Q$. Simple algebra dictates that

$$\left|Q^{n}\cdot P\right|=\left|Q^{n}\right|$$

Hence,

$$\left|Q^{n+1}\right| = \left|Q^{n} \cdot P\right| - \left|Q^{n} \cdot \Delta\right| = \left|Q^{n}\right| - \left|Q^{n} \cdot \Delta\right|$$

Since $Q^n \cdot \Delta$ has only positive and zero elements, this means that $|Q^n \cdot \Delta| > 0$. Therefore,

$$|Q^{n+1}| < |Q^n|$$
 $(c-1)/c^2 \cdot |Q^n_{c+1}| \ge (c-2)/(c-1)^2 \cdot |Q^n_c|$

As

$$p_f \ge 1 - (C-2)/(C-1)^2 \cdot |Q^n|$$

This means that p_f is an increasing function of n. For example, given C = 4,

$$|Q \cdot \Delta| = 4 \cdot a^2$$

Hence,

$$\left|Q^{2}\right| = \left|Q\right| - 4 \cdot a^{2} < \left|Q\right|$$

Lemma 3. It turns out that the probability that the capacity of a link will be optimal is greater than or equal to

$$p_{c} \geq \min_{c=1,...C} \left\{ 1 - (c-2)/(c-1)^{2} \cdot |Q_{c}^{n}| \right\}$$

= 1 - (C-2)/(C-1)^{2} \cdot |Q_{c}^{n}| (6)

Note that p_c is the probability of achieving the optimal capacity and $Q_c = Q_f$. But if we assume learning, then Q_f and Q_c will change as a function of n, in which case they will not necessarily evolve in the same way. Observe that the capacity of a link must be greater than the flow through that link; otherwise the average time latency shown in Eqn (1) is ill defined. If a flow is j, then the capacity ranges from j+1 to C. If we shift the capacity to the left by j, we get cranging from 1 to C - j. Since $j \ge 0$, the largest value for c is C. Since the largest value of c is C and

$$(c-1)/c^2 \cdot |Q_{c+1}^n| \ge (c-2)/(c-1)^2 \cdot |Q_c^n|$$

for all c, as proved below, we can assert Lemma 3.

Proof of Lemma 3. We will proceed by induction on n. The first step is to prove that the lemma holds for n = 1. That is,

$$(c-1)/c^2 \cdot |Q_{c+1}| \ge (c-2)/(c-1)^2 \cdot |Q_c|$$

Since $(c-1)/(c) \ge (c-2)/(c-1)$, we only need to show that $1/c \cdot |Q_{c+1}| \ge 1/(c-1) \cdot |Q_c|$. This can be established by observing that $|Q_c| = (c - 3 + 4/3)$.

Now we assume that this is true for all k = 1, ..., nand prove for n+1. We will show that this is true when c is odd. A similar proof can be shown when c is even.

Assume that *c* is odd. Let $Q_c^n = \left[\overline{d}_1^n; \overline{d}_2^n; ...; \overline{d}_{c-1}^n\right]$ where \overline{d}_i^n is the *i*th column of Q_c^n and $Q_{c+1}^n = \left[\overline{e}_1^n; \overline{e}_2^n; ...; \overline{e}_c^n\right]$ where \overline{e}_i^n is the *i*th column of Q_{c+1}^n . Note that we have removed the boundary rows and columns of Q_c^n and Q_{c+1}^n whose elements are 0. This will not affect the proof. Q_c^n obeys a recursion:

$$Q_{c}^{n} \cdot Q_{c} = a \cdot \begin{bmatrix} \overline{d}_{1}^{n} + \overline{d}_{2}^{n}; \overline{d}_{1}^{n} + \overline{d}_{2}^{n} + \overline{d}_{3}^{n}; \\ \overline{d}_{2}^{n} + \overline{d}_{3}^{n} + \overline{d}_{4}^{n}; ...; \overline{d}_{c-2}^{n} + \overline{d}_{c-1}^{n} \end{bmatrix}$$
(7)

 Q_{c+1}^n obeys a recursion similar to the one above. Applying recursion and induction repeatedly we get p inequalities where $p = \left\lfloor \frac{c}{2} \right\rfloor$. Each time, the new inequality is obtained by removing the first term and the last term both on the LHS and on the RHS of the previous inequality.

$$\begin{aligned} &\frac{1}{c} \cdot \left(\left| \vec{e}_{2}^{n-1} \right| + \ldots + \left| \vec{e}_{c-1}^{n-1} \right| \right) \geq \frac{1}{c-1} \cdot \left(\left| \vec{d}_{2}^{n-1} \right| + \ldots + \left| \vec{d}_{c-2}^{n-1} \right| \right) \\ &\frac{1}{c} \cdot \left(\left| \vec{e}_{3}^{n-2} \right| + \ldots + \left| \vec{e}_{c-2}^{n-2} \right| \right) \geq \frac{1}{c-1} \cdot \left(\left| \vec{d}_{3}^{n-2} \right| + \ldots + \left| \vec{d}_{c-3}^{n-2} \right| \right) \\ & \dots \end{aligned}$$

$$\frac{1}{c} \cdot \left(\left| \vec{e}_{p}^{n-p} \right| + \left| \vec{e}_{p+1}^{n-p} \right| + \left| \vec{e}_{p+2}^{n-p} \right| \right) \\
\geq \frac{1}{c-1} \cdot \left(\left| \vec{d}_{p}^{n-p} \right| + \left| \vec{d}_{p+1}^{n-p} \right| + \left| \vec{d}_{p+2}^{n-p} \right| \right) \tag{8}$$

$$\frac{1}{c} \cdot \left(\left| \vec{e}_{p}^{n-p-1} \right| + 2 \cdot \left| \vec{e}_{p+1}^{n-p-1} \right| + \left| \vec{e}_{p+2}^{n-p-1} \right| \right) \\ \geq \frac{1}{c-1} \cdot \left(\left| \vec{d}_{p}^{n-p-1} \right| + \left| \vec{d}_{p+1}^{n-p-1} \right| \right)$$
(9)

where $|\vec{x}|$ is the sum of all elements of the vector

 \overline{x} . The lemma is true if the first inequality is true. But the first inequality is true if the second inequality is true. Repeating the argument tells us that the lemma is true if the last inequality is true. Again, by induction, Eqn (8) is true when we replace n-p with n-p-1:

$$\frac{1}{c} \cdot \left(\left| \vec{e}_{p}^{n-p-1} \right| + \left| \vec{e}_{p+1}^{n-p-1} \right| + \left| \vec{e}_{p+2}^{n-p-1} \right| \right) \\
\geq \frac{1}{c-1} \cdot \left(\left| \vec{d}_{p}^{n-p-1} \right| + \left| \vec{d}_{p+1}^{n-p-1} \right| + \left| \vec{d}_{p+2}^{n-p-1} \right| \right)$$
(10)

Combining Eqns (9) and (10), we get:

$$\frac{1}{c} \cdot \left(\left| \vec{e}_{p}^{n-p-1} \right| + 2 \cdot \left| \vec{e}_{p+1}^{n-p-1} \right| + \left| \vec{e}_{p+2}^{n-p-1} \right| \right)$$

$$\geq \frac{1}{c} \cdot \left(\left| \vec{e}_{p}^{n-p-1} \right| + \left| \vec{e}_{p+1}^{n-p-1} \right| + \left| \vec{e}_{p+2}^{n-p-1} \right| \right)$$

$$\geq \frac{1}{c-1} \cdot \left(\left| \vec{d}_{p}^{n-p-1} \right| + \left| \vec{d}_{p+1}^{n-p-1} \right| + \left| \vec{d}_{p+2}^{n-p-1} \right| \right)$$

Hence the proof is complete because we have shown that the inequality (9) is true.

Corollary. Combining the result of Lemma 1 to that of Lemma 3, we obtain the second main result of this paper, the lower bound to the probability of finding the optimal solution in a network which has e links:

$$p \ge \left(1 - \frac{C - 2}{(C - 1)^2} \cdot \left|Q_C^n\right|\right)^s \cdot \left(1 - \frac{C - 2}{(C - 1)^2} \cdot \left|Q_C^n\right|\right)^e$$

$$= \left(1 - \frac{C - 2}{(C - 1)^2} \cdot \left|Q_C^n\right|\right)^{e+s}$$
(11)

Proof of Corollary. The probability of finding the optimal solution is the product of the probabilities that each path carries the optimal flow (provided by Eqn (3)) and the probabilities that each link has the optimal capacity (provided by Eqn (6)). That is, following the inequality sign in Eqn (11), the first factor is the lower probabilistic bound of finding the optimal flows where s is the total number of paths between all pairs of nodes, while the second factor is the lower probabilistic bound of finding the optimal capacities for e links.

Fig 3 below shows the probability of achieving the optimal solution as a function of the number of runs. The C value means the flow through each

link ranges from 0 to 20, 0 to 21 or 0 to 22. Fig 3 assumes the network shown on the LHS of Fig 1, i.e. there are ten links (e=10) and ten pairs of nodes. Assume five paths per pair of nodes yields $s = 50 = 10 \cdot 5$. Based on Eqn (11), the lower bound for the probability of finding the optimal solution is:

$$p \ge (1 - (C - 2)/(C - 1)^2 \cdot |Q_C^n|)^{60}$$

CONCLUSION

We have described a new agent-based algorithm that allows optimizing an objective function that depends both on the flow and the capacity of each link and which satisfies the traffic matrix constraint. In addition, we have derived a novel rate of convergence for this algorithm when assuming no reinforcement learning. We believe that we can further derive the rate of convergence when reinforcement learning is imposed. In a future paper, we will present this more complex derivation and analyze the time latency of an existing network known as the Networked Underwater Warfare Technology Demonstration Program, currently being conducted at Defence Research and Development Canada - Atlantic.



Fig 3 – Probability of achieving the optimal solution as a function of number of runs.

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HIERARCHIC GENETIC SCHEDULER OF INDEPENDENT JOBS IN COMPUTATIONAL GRID ENVIRONMENT

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ABSTRACT

In this work we present an implementation of Hierarchic Genetic Strategy (HGS) for Independent Job Scheduling on Computational Grids. In our formulation of the scheduling problem, makespan and flowtime parameters are simultaneously optimized. The efficient assignment of jobs to machines that optimizes both objectives is crucial for many Grid systems. The objective of this work is to examine several variations of HGS operators in order to identify a configuration of operators and parameters that works best for the problem. Differently from classical GA algorithms, which maintain only an unstructured population of individuals, HGS performs by many small populations enabling a concurrent search in the optimization domain. From the experimental study we observed that HGS implementation outperforms existing classical GA schedulers for most of considered instances of a static benchmark for the problem.

INTRODUCTION

Grid technologies have primarily emerged for scientific and technical work, where geographically distributed computers, linked through Internet, are used to create virtual supercomputers of vast amount of computing capacity which enables to solve complex problems from e-Science domain. During the past years Grid Computing has shown its feasibility to achieve breakthroughs in meteorology, physics, medicine and other computingintensive fields. Grid computing is still in the development stage, and most projects are still from academia and large IT enterprises; it has however developed very quickly and more and more scientists are currently engaged to solve many challenges in Grid Computing. One important challenge in Grid computing is the design and implementation of efficient Grid schedulers as a basis for the development of high performance Gridenabled applications. Scheduling problem in Grid systems can be seen as a family of problems, depending on the way how the problem is formalized (realistic vs. simulated), the number of objectives to optimize (single vs. multi-objective), the environment (static vs. dynamic), processing mode (immediate vs. batch), job dependencies (independent vs. dependent), etc.

In this work we consider the scheduling problem formulation, referred to as Independent Job Scheduling, in which: (a) expected time to compute values of jobs in machines are known; (b) two objectives, namely makespan and flowtime are optimized (bi-objective optimization); (c) the environment is dynamic; (d) jobs are processed in batch mode; and, (d) jobs are independent (or loosely coupled).

Independent job scheduling appears usually in data intensive computing such as data mining and massive processing applications. For this class of Grid-enabled applications, batch mode is appropriate given that such application manage voluminous data, could run periodically and also because large amount of data have to be transferred, replicated and accessed by the applications. In such case, jobs or applications are grouped in *batches* and scheduled as a group. Batch mode scheduling methods are simple and yet powerful heuristics that are distinguished for their efficiency by taking better advantage of job and resource characteristics since they dispose of the time interval between two successive activations of the batch scheduler.

The objective in this work is to design and implement batch schedulers based on a family of dependent genetic processes enabling a concurrent search in the optimization domain. We defined a *Hierarchic Genetic Scheduler (HGS-Sched* which is based on the Hierarchical Genetic Strategy (HGS) defined by (Kołodziej et al., 2001).

HGS is an effective tool for solving continuous global

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optimization problems with multimodal and weakly convex objective functions. It was successfully applied to some practical engineering problems, for example for the estimation of the geometric errors of the Coordinate Measure Machine (Kołodziej et al., 2004). The successful applications of HGS make it a candidate algorithm for the design of efficient batch schedulers in Grid systems for which time efficiency and high quality planning are crucial.

The rest of the paper is organized as follows. We introduce the scheduling problem and its definition in Section "STATEMENT OF THE PROBLEM". Definitions of HGS-Sched procedures and a short description of applied genetic operators are given in Section "HIERARCHIC GENETIC SCHEDULER FOR GRID SYSTEMS". Section "EXPERIMENTAL STUDY FOR STATIC SCHEDULING" contains an experimental analysis of the performance of HGS-Sched and some selected singe-population genetic algorithms for the benchmark of static scheduling. The paper ends in Section "CON-CLUSIONS" with some final remarks.

STATEMENT OF THE PROBLEM

Scheduling of jobs to Grid resources is indispensable for Computational Grids to ensure high performance Gridenabled applications. Notice that the scheduling impacts, on the one hand, on Grid resource utilization, the efficiency of Grid applications and also on the QoS of the Grid system. Unlike traditional schedulers of conventional distributed systems, centralized Grid (global) schedulers have to manage the inherent heterogeneous structure of the Grid, the existence of local schedulers in different organizations or resources and the possible restrictions of the jobs to be scheduled (restrictions on the resources needed to complete the job, transmission cost, etc.).

In this work we consider the problem formulation based on the Expected Time to Compute matrix model. In this model (Ali et al., 2000), it is assumed that we know:

- The estimation or prediction of the computational load of each job (e.g. in millions of instructions). This information is usually given from job specification or is extracted from execution traces.
- The computing capacity of each resource (e.g. in millions of instructions per second, MIPS).
- The estimation of the prior load of each one of the machines. Machines in the system could be idle (in such case the prior load is zero) or could be running some job and have a pending queue of jobs. In this later case, the prior load is equal to the current load of the machine plus the computing load due to the execution of the pending jobs in the queue.
- The entries of the *ETC* matrix, denoted by $ETC[\tilde{j}][\tilde{m}]$ indicates the expected time to compute

job \tilde{j} in resource \tilde{m} . A simple way to compute $ETC[\tilde{j}][\tilde{m}]$ entry is by dividing the computing load of a job \tilde{j} by the computing capacity of a machine \tilde{m} .

Further, the bi-objective optimization model is considered for the problem, namely the minimization of *makespan* and *flowtime*, where $F_{\tilde{j}}$ denotes the time when job \tilde{j} finalizes and *Sched* is the set of all possible schedules; the two objectives are integrated into a single objective function.

$$makespan = \min_{S_i \in Sched} \{ \max_{\tilde{j} \in Jobs} F_{\tilde{j}} \}$$
(1)

$$flow time = \min_{S_i \in Sched} \{ \sum_{\tilde{j} \in Jobs} F_{\tilde{j}} \} .$$
 (2)

Makespan expresses the performance of a Grid systems; the smaller the values of makespan, the closer to the optimal is the scheduling of jobs to Grid resources, and hence, the faster is the executions of jobs in the Grid system. On the other hand, flowtime, expresses the response time to the submitted job execution requests of Grid users and therefore, flowtime is usually considered as QoS criterion in Grid systems.

HIERARCHIC GENETIC SCHEDULER FOR GRID SYSTEMS - (HGS-Sched)

Many kinds of genetic algorithms defined for the scheduling problems (see Braun et al. (2001), Xhafa et al. (2007b)) can be implemented as *the law of evolution*, which governs the progression from one generation to the next. GA's objective is to explore as much as possible the solution space using a population of individuals and to find the best solution for the problem at hand. Due to the large size of the solution space, an intelligent space exploration is thus critical for GAs and is usually achieved through the use of genetic algorithms. It should be noted that classical GAs running in sequential setting define a single evolutionary process.

The main idea of HGS-Sched is running a set of dependent evolutionary processes. This dependency relation has a tree structure with the restricted number of levels. Every single process "creates" a branch in this structure and can be defined as a sequence of evolving populations. The core of the structure governs the search procedures and it is active until the stopping criterion for the whole strategy is satisfied. The HGS-Sched mechanism is different than the mechanism of other hierarchical and branching schedulers presented in the literature (see (Brucker , 2007) for example).

For each branch we define a *degree* parameter, denoted by $j \in \mathbb{N}$, the value of which corresponds to the accuracy of the search in this branch. There is a unique branch of the lowest degree 0 called *root*. The processes of lower degree (close to the root) represent chaotic search with a low accuracy. They detect the promising regions in



Figure 1: An example structure of HGS-Sched after execution of 3 metaepochs

the optimization landscape, in which more accurate processes of higher order are activated. A new branch could be created after running a metaepoch in the parental one.

Let us denote by $P_{i,j}^e$ populations evolving in branches of the different degrees, where $e \in \mathbb{N}$ is the global metaepoch counter, j, $(j \in \{1, \ldots, M\}, M \in \mathbb{N})$ is a degree of the branch, M is the maximal degree of a branch and i-is the unambiguous branch identifier, $i = (i_1, \ldots, i_M)$, $i_h = 0$ for h > j, which describes the "history of creation" of the given branch (Schaefer, and Kołodziej).

A k –periodic metaepoch $M_k, (k \in \mathbb{N})$ is a discrete evolution process terminating after k generations by the selection of the best adapted individual. The outcome of the metaepoch started from the population $P_{i,j}^e$ may be denoted by:

$$M_k(P_{i,j}^e) = \left(P_{i,j}^{e+l}, \hat{x}\right);\tag{3}$$

for some i, j, where $P_{i,j}^{e+l}$ is the resulting population and \hat{x} is the best adapted individual in the metaepoch.

An example structure of HGS-Sched is shown in Figure 1.

The algorithm starts from an initial population generated (usually randomly) for the root. A procedure of activation of a new process of higher degree is called a *Sprouting Operation*. It is performed conditionally, according to the outcome of a *Branch Comparison Operation*. The definitions of these operations together with the description of all operators implemented in the genetic engine of HGS-Sched are presented in the rest of this section.

Genetic Engine in HGS-Sched Branches

We used in our implementation a genetic algorithm template, defined in Algorithm1 below, for the description of a general framework of the genetic engine in HGS-Sched branches.

Similar template can be found in (Xhafa et al., 2007b).

Algorithm 1 Genetic engine template

Generate the initial population P^0 of size μ ; Evaluate P^0 ; while not termination-condition do Select the parental pool T^t of size λ ; $T^t := Select(P^t)$; Perform crossover procedure on pars of individuals in T^t with probability $p_c; P_c^t := Cross(T^t)$; Perform mutation procedure on individuals in P_c^t with probability p_m ; $P_m^t := Mutate(P_c^t)$; Evaluate P_m^t ; Create a new population P^{t+1} of size μ from individuals in P^t and/or $P_m^t; P^{t+1} := Replace(P^t; P_m^t)$ t := t + 1; end while return Best found individual as solution;

Representations of Individuals and Genetic Operators

We used two methods of encoding of individuals for the representations of solutions of scheduling problems: *direct* and *permutation-based* representation (Xhafa et al., 2007b). The advantage in using two representations is that different families of operators can be defined for each of them, increasing thus the possibilities for operator configurations in GAs.

In **direct representation** solutions are encoded into a schedule vector $x = [x_1, \ldots, x_n]^T$, where $x_i \in [1, m]$ for $i = 1, \ldots, n, n$ is the number of jobs and m is the number of machines. Coordinate i indicates the number of machine, to which job i is assigned.

The following vector $[1, 2, 1, 1, 3, 1, 2, 2, 3, 3]^T$ is a simple example of the schedule for 3 machines and 10 jobs.

In **permutation-based** representation first we define for each machine a sequence of jobs assigned to it, then we concatenate all obtained sequences into one ordered sequence (a permutation) of coordinates of job-machine allocation vector. It is also necessary to define an additional vector of size m with number of jobs assigned to the machines. An individual's chromosome is defined as a pair of vectors:

$$x = (u; v), u = [u_i, \dots, u_n]^T, v = [v_1, \dots, v_m]^T$$
 (4)

where $u_i \in [1, ..., n]$ and $v_j \in [1, ..., n]$.

The permutation-based representation for the schedule from the above example is as follows: $([1,3,4,6,2,7,8,5,9,10]^T; [4,3,3]^T$. As can be seen, to machine 1 are assigned 4 jobs (1,3,4,6), to machine 2 are assigned 3 jobs (6,2,7), and so on.

Note that in the first representation many coordinates can have the same value, what does not cause in u in the permutation-based encoding. We applied both encoding methods in our work. We used direct representation for the individuals in base populations of the GA algorithm denoted by P^t in Algorithm 1. The permutation-based representation is necessary for running some crossover procedures defined below.

As the fitness function we define the bi-objective for scheduling given by the following formula:

$$fitness := makespan + flow time,$$
 (5)

which is minimized in our work.

The initial population for the root of the HGS-Sched structure is selected randomly. The processes of higher degrees start from the populations obtained as the outcomes of the *Sprouting Operator* defined in the next section.

The genetic procedures used in a main loop of Algorithm 1 are selected from the following set of operators:

- Selection operators: Linear Ranking Selection, N-Tournament Selection;
- **Crossover operators:** One Point Crossover, PMX, OX, CX;
- Mutation operators: Move, Swap, Rebalancing;
- **Replacement operators:** Simple Generational, Elitist Generational.

All those operators are defined in GA algorithm for the problem in (Xhafa et al., 2007b). We briefly describe here the mutation operators whose definition is more problem dependent; the selection and replacement operators are defined as usually in GAs. Three definitions are considered for the mutation operator. Move moves a job from one machine to another one. Although the job can be appropriately chosen, this mutation strategy tends to unbalance the number of jobs per machine. The mutation *Swap*, keeps the number of jobs per machines unchanged by swapping two jobs in two different machines. Finally, *Rebalancing* makes use of the load balancing technique.

HGS-Sched Branching Operators

To extend the tree structure of HGS-Sched we introduced two branching operators: *HGS-Sched Sprouting Operator* (SO) and *Branch Comparison Operator* (BC).

The *SO* operator, which is responsible for creation of new branches of higher degree, is defined by the following formula:

$$SO(P_{i,j}^e) = (P_{i,j}^e, P_{i',j+1}^0),$$
 (6)

where \hat{x} is the best adapted individual found in the parental branch $P_{i,j}^e$ after execution of *e*-th metaepoch, $P_{i',j+1}^0$ is an initial population for a new branch of degree j + 1 and $i' = (i_1, \ldots, i_{j-1}, 1, 0, \ldots, 0)$.

The individuals in population $P_{i',j+1}^0$ are selected from the s_j -neighborhood $(1 \le s_j \le n)$ of the solution \hat{x} defined in the following way. Let A_{s_j} be the operator which "cuts out" a s_j -length prefix from a given chromosome x. It is defined as follows:

$$A_{s_j}(x) = \tilde{x}, |\tilde{x}| = s_j, |x| \ge s_j, \tag{7}$$

where |x| = n denotes the length of x. The s_j neighborhood of solution x contains all individuals which can differ from x by the $(n-s_j)$ -length suffixes in their genotypes. It can be achieved by the permutation of jobs in the suffix in the permutation-based representation or job transfers to another machines in the suffix in the case of direct representation of individuals.

The values of s_j are different for branches of the different degrees. These parameters are calculated using the following formula:

$$s_j = s^j \cdot n, \tag{8}$$

where $s \in [0, 1]$ is a global strategy parameter called *neighborhood parameter*, *j*- the branch degree, *n*- the number of jobs.

The sprouting operation can be activated or not, depending on the outcome of *Branch Comparison* operator $BC: Q \rightarrow \{0, 1\}$ defined below:

$$BC(X, Y, s_j) = \begin{cases} 1, & \exists x \in X, \exists y \in Y : \\ & A_{s_j}(x) = A_{s_j}(y) \\ 0, & \text{otherwise}, \end{cases}$$
(9)

where $Q = \{(X, Y, s_j)\}$ and X, Y- are the populations in branches of degrees j and j+1 respectively. In the case presented in Figure 1 the value of *BC* is 1. The value 0 means that the parental branch cannot sprout a branch, which is similar to existing branches of the same degree. This operator is activated after execution of at least two metaepochs in the root.

The codes of procedures for those two operators are very similar to the codes of *SO* and *PC* procedures for HGS, which can be found in (Kołodziej et al., 2001).

EXPERIMENTAL STUDY FOR STATIC SCHEDULING

We have conducted a first experimental evaluation of the HGS implementation for the problem. Although our ultimate goal is to test and evaluate the HGS-based scheduler in a dynamic environment, we found it useful to initially use a static benchmark for evaluating the HGS implementation and compare it with state-of-the-art GAs results for the scheduling problem.

Our experiments were performed for benchmark of static instances for scheduling problem classified into 12 types of ETC matrix, according to three parameters: job heterogeneity, machine heterogeneity and consistency. Each instance consists of 512 jobs and 16 machines and is labelled by u_x -yyzz.0 like in (Braun et al., 2001) and (Xhafa et al., 2007b):

- u means uniform distribution (used in generating the matrix).

- x means the type of consistency (c-consistent, iinconsistent and s means semi-consistent). An ETC matrix is considered consistent when, if a machine $m_{\tilde{i}}$ executes job \tilde{j} faster than machine $m_{\tilde{j}}$, then $m_{\tilde{i}}$ executes all the jobs faster than $m_{\tilde{j}}$. Inconsistency means that a machine is faster for some jobs and

Table 1: HGS-Sched global parameters values

Parameter	Value
degrees of branches (j)	0 and 1
$period_of_metaepoch - (k)$	200
$nb_of_metaepochs$	10
neighborhood parameter - (s)	0.5
$mut_prob(0)$	0.4
$mut_prob(1)$	0.2
cross_prob	0.8

slower for some others. An ETC matrix is considered semi-consistent if it contains a consistent submatrix.

- yy indicates the heterogeneity of the jobs (hi means high, and lo means low).

- zz indicates the heterogeneity of the resources (*hi* means high, and *lo* means low).

The benchmark tries to capture different real Grid scenarios by combining different characteristics of the Grid systems such as computing consistency, heterogeneity of resources and jobs.

The values of HGS-Sched parameters for all tests are given in Table 1.

The parameter $nb_of_metaepochs$ defines a global stop criterion for the whole strategy, which is the maximal number of metaepochs run in the root of the structure. We denoted by $mut_prob(j)$ the probability of mutation in the branch of degree j $(mut_prob(0)$ and $mut_prob(1)$ are the probabilities of mutation for the root and the branches of degree 1 respectively). We assume that the probability of crossover, denoted by $cross_prob$, takes the same value in the branches of all degrees. The initial population of the root was created by a uniform random generator and linear ranking method was used as selection procedure.

We conducted the experimental study into two steps. First, we tried to find an appropriate combination of genetic operators for HGS-Sched. Then, in the second step, we made a short comparison analysis of the performances of our algorithm and GA-based schedulers presented in (Braun et al., 2001) and (Xhafa et al., 2007b).

Tuning of Genetic Operators for HGS-Sched

A simple tuning process of genetic operators for HGS-Sched was performed for one instance of ETC matrix labeled by u_c_hihi.0. The sizes of populations in root and sprouted branches of degree 1 were 50 and 18, respectively. The intermediated populations consisted of 48 and 16 individuals in the case of Elitist replacement and 38 and 14 in the case of Simple Generational replacement. Each experiment was repeated 30 times under the same configuration of operators and parameters and the average makespan and flowtime values were computed.

Table 2 shows the results obtained for four types of crossover operators and Rebalancing mutation. CX and

Table 2: Comparison of crossover operators for makespan and flowtime values.

Operator Average Makespan		Average Flowtime	
PMX	8147446.46338	1096287320.223	
OX	9283953.76642	1249786030.004	
CX	7696260.50065	10413560968.452	
OnePoint	7696439.32214	10413530955.129	

Table 3: Comparison of mutation operators for makespan and flowtime values.

Operator	Average Makespan	Average Flowtime
Move	8853148.607664	1087530440.192
Swap	19031484.397466	2283034176.802
Rebalancing	7696260.50065	10413560968.452

OnePoint methods are more effective than OX and PMX, while the differences in makespan and flowtime values calculated for them are minor. We decided to choose the CX operator for our strategy engine, based on the results of similar analysis presented in (Xhafa et al., 2007b).

The results of the comparison analysis of the performance of three mutation operators are reported in Table 3. We combined them with CX procedure. Rebalancing method outperforms significantly Move and Swap mutations.

The values of fitness components calculated for two considered replacement procedures are given in Table 4. The appropriate combination of genetic operators for HGS-Sched is completed with the Elitist Generational replacement method due its better performance.

Comparison Analysis of Genetic-Based Schedulers

Once fine tuned, the operators and parameters were used for a comparison analysis of three genetic algorithms, namely our implementation of HGS-Sched with GA schedulers defined in (Braun et al., 2001) and (Xhafa et al., 2007b). It should be noted that the GA in (Xhafa et al., 2007b) outperformed the GA in (Braun et al., 2001) and, it was thus interesting to see the performance of our HGS-Sched with respect to the two GA algorithms.

All 12 instances of ETC matrix were used in our experimental study. In fact, the objective was not only to study the performance of the HGS-Sched but also to see its behavior regarding three group of instances: consistent, semi-consistent and inconsistent. Conclusions in

Table 4: Comparison of applied replacement operatorsfor makespan and flowtime values.

Operator	Average Makespan	Average Flowtime
Generational	7744052.84523	1047480700.341
Elitist Generational	7696260.50065	10413560968.452

this regard are interesting when the scheduler is to be designed for certain type of Grid infrastructures.

In order to make a fair comparison we considered that it is important to use not only the execution time, which is an arbitrary stopping condition, but also the amount of work done by the algorithm. The objective was thus to observe the performance of the algorithms, within the same amount of time, even though they use different genetic operators and parameter values.

We defined the work of GA in Eq. (10).

$$W = (mut_prob + cross_prob) \times \\ \times pop_size \times nb_of_generations$$
(10)

For HGS-Sched parameter W is calculated as given in Eq. (11).

$$W = \begin{bmatrix} (mut_prob(0) + cross_prob) \times pop_size(0) + \\ + \sum_{j=1}^{M} ((mut_prob(j) + cross_prob) \times \\ \times pop_size(j) \times nb_br(j)) \end{bmatrix}$$

×period_of_metaepoch×
×nb_of_metaepochs (11)

where:

- M is the maximal degree of the branch,
- nb_br(j) is the number of sprouted branches of degree j,
- pop_size(j) denotes the size of population in the branch of degree j.

Based on Eqs. (10) and (11), the amount of work calculated for analyzed schedulers are as follows:

- for GA in (Braun et al., 2001): W = (0.4 + 0.6) * 200 * 1000 = 200000,
- for GA in (Xhafa et al., 2007b): W = (0.4 + 0.8) * 68 * 2500 = 240000, and
- for HGS-Sched: W = W = ((0.2 + 0.8) * 8 * 12 + (0.4 + 0.8) * 28) * 200 * 10 = 259200.

As can be seen from the above values, the three algorithms perform a similar amount of work, ensuring thus a fair comparison between them.

Comparison of makespan values. We present in Table 5 the makespan values obtained by the three genetic algorithms under study.

From the results in Table 5 we can observe that HGS-Sched outperforms the GA by Braun et al. for all but one instance and the GA by Xhafa et al. for 75% of considered instances. Notice that HGS-Sched performs better for consistent and semi-consistent ETC matrices. This observation is useful in considering HGS-Sched as a basis for Grid scheduler that have consistent computing features. It is also interesting to observe that HGS-Sched

Table 5: Comparison of best makespan values for threegenetic algorithms. Best results are shown in bold

Instance	Braun et al.	Xhafa et al.	HGS-Sched
u_c_hihi	8050844.500	7610176.437	7606401.235352
u_c_hilo	156249.200	155251.196	155063.78363
u_c_lohi	258756.770	248466.775	248059.043238
u_c_lolo	5272.250	5226.972	5215.044607
u_i_hihi	3104762.500	3077705.818	3077989.170045
u_i_hilo	75816.130	75924.023	76122.941623
u_i_lohi	107500.720	106069.101	108646.831972
u_i_lolo	2614.390	2613.110	2620.150313
u_s_hihi	4566206.000	4359312.628	4343467.785157
u_s_hilo	98519.400	98334.640	98179.968964
u_s_lohi	130616.530	127641.889	127065.766276
u_s_lolo	3583.440	3515.526	3575.692663

Table 6: Best flowtime values for benchmark instances (in arbitrary time units). Best results are shown in bold.

Instance	Xhafa et al.	Xhafa et al.	HGS-Sched
	Steady State GA	Struggle GA	
u_c_hihi	1048333229	1039048563	1040162825.157
u_c_hilo	27687019.4	27620519,	27578766.613549
u_c_lohi	34767197.1	34566883,8	34530865.9457
u_c_lolo	920475.17	917647,31	916896.056194
u_i_hihi	378010732	379768078	358850693.7164
u_i_hilo	12775104.7	12674329,1	12665322.029
u_i_lohi	13444708.3	13417596,7	12880192.58278
u_i_lolo	446695.83	440728,98	441201.6681
u_s_hihi	526866515	524874694	522084156.1341
u_s_hilo	16598635.5	16372763,2	16419442.90678
u_s_lohi	15644101.3	15639622,5	15370602.53526
u_s_lolo	605375.38	598332,69	601220.872348

performed consistently and robustly, that is, it achieved high quality schedulers for the same type of examples in all different executions carried out for this experimental study.

Comparison of flowtime values. We present in Table 6 the flowtime values obtained with the Steady State GA by Xhafa et al., Struggle GA presented in (Xhafa et al., 2008) and HGS-Sched algorithm (Braun et al. did not report values for flowtime parameter).

From the results in Table 6 we conclude that HGS-Sched outperforms Steady State GA for all types of ETC matrices and it is better than Struggle GA in 8 instances. In the case of flowtime, HGS-Sched performed consistently for all three groups of instances (consistent, semiconsistent and inconsistent ETC matrices).

Results of Summative Evaluation. The results of the experimental study showed that HGS-based scheduler performs better that GA-based schedulers reported for the problem in the literature for both makespan and flow-time minimization. Although the experimental study has been conducted on a small set of instances and of rather small sizes, HGS algorithms can be considered suitable for the design of Grid schedulers. Regarding the effect of Grid characteristics (features of ETC matrix) such as consistency of computing and heterogeneity, the most

significant differences in the obtained results for HGS-Sched and GAs were observed for the instances of inconsistent ETC matrices, where the reduction of makespan by the hierarchic scheduler was not so effective.

CONCLUSIONS

In this work we have presented the implementation of Hierarchic Genetic Strategies (HGS) for Independent Job Scheduling on Computational Grids for which both makespan and flowtime parameters are simultaneously optimized. Achieving high quality planning of jobs into machines is crucial for Grid systems due to their heterogenous and dynamic nature. To this end, we have examined several variations of HGS operators in order to identify a configuration of operators and parameters that works best for the problem aiming at the design of efficient batch schedulers. The HGS implementation was experimentally studied using a known benchmark of static instances for the problem and the obtained results were compared with those of two other GA schedulers from the literature. From the experimental study we observed that HGS implementation outperforms existing classical GA implementations in the literature for most of considered instances of a static benchmark for the problem. In particular, HGS performed very well for instances representing features of consistent and semiconsistent computing environments.

In our future work we plan to study the performance of the HGS scheduler using the Grid simulator in Xhafa et al. (2007a). We would also like to design an interface for our HGS scheduler for its application to real Grid environments.

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Modelling Granule Dependent Information in Vehicular Ad Hoc Networks

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1. Introduction

This paper presents a novel simulation model which incorporates traffic simulation model and a Vehicular Ad Hoc networking model to achieve temporal and geo-spatial information granules formations simulation for the vehicles in the urban traffic networks in real-time using the concepts and techniques of Granular Computing theory.

The Granular Computing theory describes the formation and the inherent features of the so-called Information Granules – basic units for aggregation of Knowledge Information carrying essential for the modelling system data. It has its formal foundations firmly based on using Fuzzy Sets, Rough Sets, Set Theory among other mathematical fields. [6][7][10][11][12][13][14][15].

We propose to combine Vehicular Ad Hoc Networks (Vanet) [1][2][3][4][5] and Granular Computing methods collaboratively to investigate the basic principles for knowledge granulation in traffic systems. We present here our achievements in determining fuzzy information granulation as localized distributed information granules within the system and we also present the identified different levels in performing system data granulation.

The overall aim of the simulation is to process in a hierarchical way traffic information data generated in the traffic system to mimic a human-like abstraction process using fuzzy set theory and granular computing.

Central to the simulation approach is the so called Car-to-Car (C2C) type of communication. It represents the possibility of cars communicating with

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) each other directly and self-organising themselves into communication networks - the so called ad-hoc networks. As well as avoiding building expensive roadside infrastructure nodes, this approach elevates on a different level the concept of distributive data generation and control. This approach illustrated on 1. however brings its own Fig challenges and problems.



Figure 1 - Vehicular Ad-hoc network formation and dissipation

We are going to utilize vehicular ad hoc networks to form a decentralized real-time environment in which data will be granulated into knowledge and used in real-time as it ripples through the network. We also assume that data is relative to time and environment. Same data can be part of different information granules at different levels. Different information granules are also relative to their strata in the hierarchy and only meaningful in current context.

The simulation assumes that each vehicle is equipped with ad-hoc communications capabilities with necessary range and there is GPS and a telematics computing device on board. Each vehicle has a map of the urban area loaded in its GPS device and vehicle is aware of its position during its travel.

The simulation of the Vehicular ad hoc network (VANET) formation is based on the ability of the telematics platform software in the vehicles themselves to form ad-hoc networks by triggering ad hoc network formations in preset geographic locations and preset times. Vehicles will have this information preloaded in their telematics platforms. The simulation of the Vanets formation then is used to obtain knowledge granules (useful pieces of traffic information) as a result of inter-vehicle communications and in-vehicle calculations. Network formation and persistence issues are built around this process. There are also two aspects to formation of the ad-hoc networks. First, roads on the inbuilt map are divided into road granules. Vehicle has the necessary calculation algorithm in its telematics system to link its position to the relevant road granule. Second element is information granulation schedule. This schedule is a mapping of all the roads times. to calculation Vehicles constantly know their current position and which road granule it is on. When there is a calculation to be performed on the road its only for the vehicles form temporary vanets only and the duration of the calculations is only for the road granules they are currently in. Those road granules geographically restrict the network boundaries. Α road may have many road granules and hence many vanets independent of each other. Each vanet performs its own calculation and obtains its own information granule result for its road

granule. We can think physically of a road granule as a road segment.

Information in the vanet formations is granulated using Granular Computing concepts. The problem domain of collaborative generation of information is fuzzy in nature. As a result the vehicles in a road segment form ad hoc networks within the pre-defined road granules and they do periodic calculations and aggregations using the formal techniques of Granular Computing and Fuzzy Granulation.

Each vehicle has an intelligent module called Network Granulation Engine. This module tracks its GPS location and matches the position to the in-built map roads and road intervals.

The Network Granulation Engine, then establishes, maintains and reestablishes all necessary ad hoc network links in accordance with the network logic and the underlying protocols.



A simulator has been developed to help with the design and the evaluation process of the model. The simulator has provided a lot of insight information into the model and during the development; it has helped to consider the model in different aspects. The development process of the simulator itself has acted as a brain storming exercise which helped to refine and shape the model.

2. Simulator Design.

Simulator has been designed to be modular to include the data from the GIS, to be an urban traffic simulator and on to superimpose onto that the network granulation engine and the information granulation engine. The urban traffic simulator generates and simulates traffic while the network aranulation engine generates geographically bound ad hoc networks and arranges the infrastructure for data communications. The information granulation engine then makes use of the data within the ad hoc network to human-centric generate fuzzy information granules.

Each network is formed reactively to do periodical calculations and a network head is selected for the duration of one cycle of calculation.

The simulator consists of three major components. The first component is the traffic simulator. This component includes a user Interface, loading and processing NTF based Ordnance Survey map data, synchronizing the data wit the Nottingham City Map and simulating traffic movement on the map. A basic traffic simulation is produced for this to form the basis of vanet based information granulation.

On top of the traffic simulator module two more components are developed as the Network Granulation Engine and the Information Granulation. The network granulation engine utilizes the road and vehicle object in the underlying traffic simulation module and granulates the roads into network granules. Each network granule maps to a physical road segment. This road granule identifies a vanet. Vanets are geographically enforced. Each vehicle knows its current position and when a calculation is triggered vehicles form vanets to perform the calculation triggered. The simulator places each vehicle from the underlying simulator into road segment objects and performs information granulation on this abstraction. Network delay is simulated as simulation cycle delay. The Information Granulator Engine takes a copy of the current state as vehicles on a road network granule, waits necessary number of cycles after which it checks vehicle positions and finds out the vehicles that have moved during this wait time and removes them from the initial state and performs the calculation on those vehicles that are still in the granule. In this way network formation latency is considered for the connection timing in the granule.

The described above component based granular structure allows different aspects of the system to be simulated independently.

One study that can be done using the simulator is the percentage of connection maintained by the granule As the model enforces size. geographically formed vanets there are two major questions regarding the infrastructure of the system that are obvious intuitively. Those are: What would be the ideal speed to maintain the highest possible connectivity during a short vanet formation and information granulation process and secondly, what will be the ideal network granule length on the road. The simulation presents the results from the simulation runs with different network granule lengths that are studied with the speed kept at 40 mph. 50 mph, 60 mph and 70 mph.

After simulating connectivity for the entire grid, first thing that came clear was the fact that road lengths in a city did not always allow for road granule lengths specified. After applying certain granule length, increase in granule length started to have less effect on connectivity as many roads did not have enough length for the specified granule lengths and also many of the roads would have some short granules left at the end. When having the combination of road end short granules and short roads, after certain value of the granule length parameter the granule length increases do not affect the connectivity in the overall system shown in Fig. 2. The total number of vehicle objects involved in each simulation is approximately: 13200. Vehicle objects are generated periodically, based on a road saturation constant and vehicles coming to the end of a road are destroyed. Vehicle speed is set as 40 mph, reflected in the simulation cycles and movement on each cycle.



Figure 2. Connectivity – Granule Length graph. Connectivity is as percentage. This is the connectivity maintained fro the duration of the network calculation.

Granule Length	Connectivity Maintained
200 meters	80.18 %
250 meters	81.86 %
300 meters	83.62 %
350 meters	83.45 %
400 meters	83.99 %
450 meters	84.59 %
500 meters	84.53 %
550 meters	84.71 %
600 meters	85.00 %
650 meters	84.86 %
700 meters	85.02 %
750 meters	85.01 %
800 meters	85.23 %

It is clearly visible from the graph that, increasing the road granule sizes does not result in equivalent linear increase in connectivity in the overall urban system.

Another variable studied in this research was the number of the road network granules in the system and how they changed with road granule length enforced. This shows a much sharper decrease initially but slows later. Longer granule lengths mean larger ad hoc network areas and more vehicles getting involved but loss of vehicles do not decrease as such. Loss of vehicles during calculation cycle happens when vehicles exits the current road network granule and enters into the next one during the calculation process. Vehicles close to the exit edge will get out of the granule during a calculation. Increasing granule length gets more vehicles involved and less percentage gets out of the edge. When the two graphs are compared this correlation can be observed.



Granule Length	Number of Granules
200 meters	2582
250 meters	2279
300 meters	2089
350 meters	1954
400 meters	1852
450 meters	1801
500 meters	1743
550 meters	1712
600 meters	1692
650 meters	1661
700 meters	1637
750 meters	1622
800 meters	1608

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3. Information Granulation

The Knowledge Granulation Engine - the data processing and knowledge generation module resides on top of the Network Granulation Engine.

While the underlying Network Granulation Engine establishes and maintains the network and deals with data flow, the Knowledge Granulation Engine processes the traffic data.

Concepts of Granular Computing are utilized for Knowledge Generation.

Ad Hoc Networks at each interval act as a coherent unit, to perform one calculation at set periods and produce a single Information Granule each time, from data received from vehicles.

This knowledge is then relayed to the Control Centre and drivers in different ways. Road side gateways are assumed to be used to obtain and relay information granules.

4. Conclusion

From our study into the two developing fields of study, Granular Computing and Vehicular Ad Hoc Networks we have come across several significant features in support of our vision. We have designed the architecture of a hierarchical real-time information system of imprecise data form the Urban Traffic System. We have established an original data processing system utilizing both fields of study.

A Vehicular Ad Hoc network level communications protocol is envisioned which will cater for the inter-vehicle intelligent knowledge generation.

Utilizing the techniques of intelligent information processing in the field Of Granular Computing, the imprecise and dynamic conditions of the Urban Traffic System can be dealt with in the way of forming a truly scalable, real-time and useful Urban Traffic Information generation and processing system. The architecture we have developed looks promising and has the potential to overcome the underlying difficulties of the imprecise and dynamic nature of the Urban Traffic System.

The proposed system architecture has been developed as a prototype solution scenario for real-time handling of infinite amount of data. This is also a roadmap and project plan for our future work.

5. Future Study

In the next stage we are going to develop a vehicular ad hoc networking communications protocol and test it.

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DESIGN OF ADVANCED TARGETING COST FUNCTION FOR EVOLUTIONARY OPTIMIZATION OF CHAOS CONTROL

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KEYWORDS

Chaos, control, optimization, evolutionary algorithms

ABSTRACT

This research deals with the optimization of the control of chaos by means of evolutionary algorithms. The main aim of this work is to show that powerful optimizing tools like evolutionary algorithms can in reality be used for the optimization of deterministic chaos control. This work is aimed on an explanation of how to use evolutionary algorithms (EAs) and how to properly define the advanced targeting cost function (CF) securing very fast and precise stabilization of desired state for any initial conditions. As a model of deterministic chaotic system, the two dimensional Henon map was used. The evolutionary algorithm Self-Organizing Migrating Algorithm (SOMA) was used in four versions. For each version, repeated simulations were conducted to outline the effectiveness and robustness of used method and targeting CF.

INTRODUCTION

The question of targeting (faster stabilization) with application to chaos control has attracted researchers since the first method for controlling of chaos was developed. The several first approaches for targeting have used special versions of OGY control scheme (Kostelich et al., 1993; Bolt and Kostelich, 1998) or collecting of information about trajectories, which fall close to desired state (Bird and Aston, 1998). Later, alot of methods were based on adaptive approach (Ramaswamy et al., 1998), center manifold targeting (Starrett, 2002) or neural networks (Iplikci and Denizhan, 2001; Iplikci and Denizhan, 2003).

Currently, evolutionary algorithms (EA) are known as powerful tools for almost any difficult and complex optimization problem. But the quality of obtained results through optimization mostly depends on proper design of the used cost function, especially when the EAs are used for optimization of chaos control. The results of numerous simulations lends weight to the argument that deterministic chaos in general and also any technique to control of chaos are sensitive to parameter setting, initial conditions and in the case of optimization, they are also extremely sensitive to the construction of used cost function.

This research utilized the Pyragas's delayed feedback control technique (Just 1999, Pyragas 1992). Unlike the original OGY control method (Ott, et al. 1990) it can be simply considered as a targeting and stabilizing algorithm together in one package (Kwon 1999). Another big advantage of Pyragas method is the amount of accessible control parameters. This is very advantageous for successful use of optimization of parameters setting by means of EA, leading to improvement of system behavior and better and faster stabilization to the desired periodic orbits. Some research in this field has been recently done using the evolutionary algorithms for optimization of local control of chaos (Richter and Reinschke, 2000; Richter, 2002). The control law in this work is based on the Pyragas method: Extended delay feedback control -ETDAS (Pyragas 1995).

This research is concerned with the investigation of the design of the advanced targeting cost functions securing the stabilization to desired UPO (unstable periodic orbit) for any initial conditions. This work presents a accumulation of research (Zelinka et al., 2007) and also collates and elaborates the experiences with application of EA to chaos control (Senkerik et al. 2006; Senkerik et al. 2007) in order to reach the better results and decrease the influence of negative phenomenon which can occur in such a challenging task, which chaos control is.

PROBLEM DESIGN

Problem selection and case studies

The chosen example of a chaotic system was the two dimensional Henon map in form (1).

$$x_{n+1} = a - x_n^2 + by_n (1) y_{n+1} = x_n$$

This work primarily consists of three case studies. All of them are focused on an estimation of three accessible control parameters for EDTAS control method to stabilize desired UPO, and a comparison of obtained results for used cost function. Desired UPOs are the following: p-1 (a fixed point) in the first case, p-2 in the second case and p-4 in the last case. All simulations were 50 times repeated for each EA version. The control method – ETDAS in the discrete form suitable for two dimensional Henon map has the form (2).

$$x_{n+1} = a - x_n^2 + by_n + F_n$$

$$F_n = K[(1 - R)S_{n-m} - x_n]$$

$$S_n = x_n + RS_{n-m}$$
(2)

where K and R are adjustable constants, F is the perturbation, S is given by a delay equation utilizing previous states of the system and m is the period of m-periodic orbit to be stabilized. The perturbation F_n in equations (2) may have an arbitrarily large value, which can cause diverging of the system outside the interval $\{-1.5, 1.5\}$. Therefore, F_n should have a value between $-F_{\text{max}}$, F_{max} and EA should find an appropriate value of this limitation to avoid diverging of the system.

The basic cost function

The proposal of the basic cost function (CF) is in general based on the simplest CF, which could be used only for the stabilization of p-1 orbit. The idea was to minimize the area created by the difference between the required state and the real system output on the whole simulation interval $-\tau_i$.

But another cost function had to be used for stabilizing of the higher periodic orbit. It was synthesized from the simple CF and other terms were added. In this case, it is not possible to use the simple rule of minimizing the area created by the difference between the required and actual state on the whole simulation interval $-\tau_i$, due to the many serious reasons, for example: degrading of the possible best solution by phase shift of periodic orbit.

This CF, is in general based on searching for desired stabilized periodic orbit and thereafter calculation of the difference between desired and found actual periodic orbit on the short time interval - τ_s (approx. 20 - 50 iterations) from the point, where the first min. value of difference between desired and actual system output is found. Such a design of CF should secure the successful stabilization of higher periodic orbit anywise phase shifted.

Furthermore, because of CF values being very close to zero, this CF also allows using of decision rule avoiding very time demanding simulations. This rule stops EA immediately, when the first individual with good parameter structure is reached, thus the value of CF is lower then the acceptable (CF_{acc}) one. Typically CF_{acc} = 0.001 at time interval $\tau_s = 20$ iterations, thus the difference between desired and actual output has value 0.0005 per iteration – i.e. successful stabilization for used control technique. This CF was also used for p-1 orbit. The CF_{Basic} has the form (3).

$$CF_{Basic} = penalization_1 + \sum_{t=\tau 1}^{\tau^2} |TS_t - AS_t|$$
(3)

where: TS - target state, AS - actual state τ_1 - the first min. value of difference between TS and AS τ_2 - the end of optimalizing interval ($\tau_1 + \tau_s$) *penalization*₁= 0 if $\tau_i - \tau_2 \ge \tau_s$; *penalization*₁= 10*($\tau_i - \tau_2$) if $\tau_i - \tau_2 < \tau_s$ (i.e. late stabilization)

The advanced targeting cost function

It was necessary to modify the definition of CF in order to decrease the average number of iteration required for the successful stabilization and avoidance of any associated problem. The CF_{Basic} is suitable for adding some term of penalization for slowly stabilizing solutions, thus it was modified for the use of all required UPOs. The CF value is multiplied by the number of iterations (*NI*) of the first found minimal value of difference between desired and actual system output (i.e. the beginning of fully stabilized UPO). To avoid problems associated with CF returning value 0 and to put the penalization to similar level as the nonpenalized CF value, the small constant (*SC*) is added to CF value before penalization (multiplying by *NI*).

Generally, there exist two possible approaches for defining the SC value. The first one capitalizes the previous simulation results with CF basic and experiences, whereas the second approach uses the automatically computed value.

The next two proposals of CF design are based on the second approach, which should avoid any problems associated with defining the value of small constant, SC in advance (especially for stabilization of higher periodic orbit). The SC value (5) is computed with the aid of power of non-penalized basic part of CF (4).

$$ExpCF = \log_{10} \left(\sum_{t=\tau 1}^{\tau^2} |TS_t - AS_t| + 10^{-15} \right)$$
(4)

$$SC = 10^{\text{ExpCF}}$$
(5)

In general, there exists two possible ways for applying the multiplication by number of iterations required for stabilization (*NI*). The first version of final design of targeting CF ($CF_{T1 - ADV}$) has the form (6). Here the sum of basic part of CF and automatically computed *SC* is multiplied by *NI*. Finally, to avoid the problems with fast stabilization, only for limited range of initial conditions, the final CF value is computed as a sum of *n* repeated simulations for different initial conditions. Consequently, the EA should find the robust solutions securing the fast targeting into desired behavior of system for almost any initial conditions.

$$CF_{T1-Adv} = \sum_{1}^{n} NI \left(SC + penalization1 + \sum_{t=\tau 1}^{\tau 2} |TS_t - AS_t| \right)$$
(6)

where: $x_{initial}$ is from the range 0.05 - 0.95 and uses step 0.1.

In the second version of targeting CF (CF_{T2 - ADV}), there is only a slight change in comparison with the previous proposal. Here the number of steps for stabilization (*NI*) multiplies only the small constant (*SC*) which is counted in the same way as in the previous case (5). This version of targeting CF (CF_{T2 - ADV}) has the form (7).

$$CF_{T2-Adv} = \sum_{1}^{n} \left((NI \cdot SC) + penalization1 + \sum_{t=\tau 1}^{\tau 2} |TS_t - AS_t| \right)$$
(7)

Graphical CF Overview

The difference between the proposed CFs can be clearly seen in Figures 1 and 2, which shows the dependence of CF values on the adjustable parameter K. Remaining parameters were set at the best values reached in optimizations; consequently the two-dimensional diagram always shows the section of global minimum. From these figures, it is obvious as to how a small change in the CF design can influence the nonlinearity and unpredictability of CF surface.



Fig. 1. Dependence of CF value on parameters K for p-2 orbit, $x_{initial} = 0.7$, CF_{T1-ADV}, R = 0.13, $F_{max} = 0.12$





Optimization algorithms

For the experiments described here, stochastic optimization algorithm SOMA (Zelinka, 2004), has been used. It was chosen because it has been proven that this algorithm has the ability to converge towards the global optimum. SOMA works with groups of individuals (population) whose behavior can be described as a competitive - cooperative strategy. The construction of a new population of individuals is not based on evolutionary principles (two parents produce offspring) but on the behavior of social group, e.g. a herd of animals looking for food. This algorithm can be classified as an algorithm of a social environment. To the same group of algorithms, particle swarm algorithm can also be put in, sometimes called swarm intelligence. In the case of SOMA, no velocity vector works as in particle swarm algorithm, only the position of individuals in the search space is changed during one generation, here called 'Migration loop'.

The rules are as follows: In every migration loop, the best individual is chosen, i.e. individual with the minimum cost value, which is called "Leader". An active individual from the population moves in the direction towards Leader in the search space. At the end of the movement, the position of the individual with minimum cost value is chosen. If the cost value of the new position is better than the cost value of an individual from the old population, the new individual appears in new population. Otherwise the old one remains for the next migration loop.

EXPERIMENTAL RESULTS

Four versions of SOMA were used for all simulations. (See Table 1). See also Table 2 for parameter set up of EA. Parameters for the optimizing algorithm were set up in such a way in order to reach the same value of maximal CF evaluations for all used versions. Each version of SOMA has been applied 50 times in order to find the actual optimum.

The primary aim here is not to show which version is better or worse but to show that the EA can in reality be used for deterministic chaos control when the targeting cost function is properly defined.

All results are shown only for variable x of two dimensional Henon map because of its form (1), where the variable y has the same values as variable x but it is only phase shifted.

Here is the list of desired UPOs:.

Henon Map with a = 1.2 and b = 0.3:

- p-1 (fixed point): $x_F = 0.8$
- p-2 orbit: $x_1 = -0.562414$, $x_2 = 1.26241$ p-4 orbit: $x_1 = 0.139$, $x_2 = 1.4495$, $x_3 = -0.8595$, $x_4 = 0.8962$

The optimization interval for p-1 orbit was $\tau_i = 100$ iterations, for higher periodic orbits (p-2 and p-4) it was mostly $\tau_i = 150$ iterations.

The ranges of all estimated parameters were these: $-2 \le K \le 2$, $0 \le F_{\text{max}} \le 0.5$ and $0 \le R \le 0.5$

Table 1: Used versions of SOMA

Index	Algorithm / Version
1	SOMA AllToOne
2	SOMA AllToRandom
3	SOMA AllToAll
4	SOMA AllToAllAdaptive

Table 2: Parameter Settings for SOMA

Parameter	ATO / ATR	ATA / ATAA
PathLength	3	3
Step	0.33	0.33
PRT	0.1	0.1
PopSize	25	10
Migrations	25	7
Max. CF Evaluations (CFE)	5400	5670

The best solution for each version of SOMA are shown in Tables 3 – 5 together with other optimization results like average number of iterations required for successful stabilization for 50 repeated simulations (Avg. IStab). The figures 3 – 11 shows the simulation of the best individual solutions for the uniformly distributed initial conditions in the range $0 < x_{initial} < 1$, and 100 samples were used in this kind of simulation

Control of chaos, p-1 orbit

The first case is focused on the stabilization of p-1 orbit. For the best individual solutions given by CF_{T1-ADV} (SOMA ATAA) and CF_{T2-ADV} (SOMA ATAA), please refer to Table 3. From the series of complex simulations depicted in Figures 3 - 5, it is obvious, that the occurrence of the phenomenon, when some best individual solutions are not suitable for complex simulation with wide range of initial conditions, whereas the remaining best solutions give excellent results, was successfully suppressed by means of usage of advanced targeting cost functions. The example of this negative phenomenon is represented by simulation of results given by CF_{Basic}. Based on obtained results, it may be stated that the control parameters estimated in the optimizations ensured very fast and precise reaching of a desired state for any initial conditions.

Table 3: Results for p-1 orbit, CF_{T1-ADV} and CF_{T2-ADV}

CF Version	CF _{T1-ADV}	CF _{T2-ADV}
Κ	-0.9977	-0.8575
$F_{\rm max}$	0.4382	0.4688
R	0.3837	0.2148
CF Val.	9.13 10 ⁻¹⁴	3.86 10 ⁻¹⁴
Avg. IStab	56	41



Fig. 3. Best solution: p-1 orbit, CF_{Basic}, SOMA ATA, complex simulation with $0 < x_{initial} < 1$, 100 samples



Fig. 4. Best solution: p-1 orbit, CF_{T1-ADV} , SOMA ATAA, complex simulation with $0 < x_{initial} < 1$, 100 samples



Fig. 5. Best solution: p-1 orbit, CF_{T2-ADV}, SOMA ATAA, complex simulation with $0 < x_{initial} < 1$, 100 samples

Control of chaos, p-2 orbit

This case is focused on the stabilization of p-2 orbit. The best results given by CF_{T1-ADV} (SOMA ATA) and CF_{T2-ADV} (SOMA ATA) are given in Table 4. The outputs of simulations are depicted in Figures 6 - 8.

The results given by CF_{T1-ADV} show the following attributes: rapid achievement of desired UPO in comparison with CF_{Basic} (on average, around 51 iterations are required), together with very poor performance of EA, i.e. the proportion of the solutions with either perfect stabilization or temporary or possibly none at all. Also, relatively considerable period doubling or oscillating in the close neighborhood of desired UPO arose (Fig 7).

In case of CF_{T2-ADV} , the two main above mentioned problems with period doubling (i.e. low-quality

stabilization) and very poor performance of EAs in finding the stabilizing securing solutions were noticeably suppressed

Table 4: Results for p-2 orbit, CF_{T1-ADV} and CF_{T2-ADV}

CF Version	CF _{T1-ADV}	CF _{T2-ADV}
K	0.3264	0.4208
$F_{\rm max}$	0.1150	0.1767
R	0.1342	0.3451
CF Val.	216.7945	5.81 10 ⁻⁹
Avg. IStab	51	133



Fig. 6. Best solution: p-2 orbit, CF_{Basic}, SOMA ATO, complex simulation with $0 < x_{initial} < 1$, 100 samples



Fig. 7. Best solution: p-2 orbit, CF_{T1-ADV} , SOMA ATA, complex simulation with $0 < x_{initial} < 1$, 100 samples



Fig. 8. Best solution: p-2 orbit, CF_{T2-ADV} , SOMA ATA, complex simulation with $0 < x_{initial} < 1$, 100 samples

Control of chaos, p-4 orbit

The last case is focused on the stabilization of p-4 orbit. See Table 5 for the results of this optimization. The simulations of the best individual solutions are depicted in Figures 9 - 11.

As a conclusion of this case study, it is possible to say that also in the case of p-4 orbit and optimizations by means of CF $_{T1-ADV}$ the phenomenon of faster targeting of desired UPO (only 84 iterations) for wide range of initial conditions occurs at the cost of poor performance of EA and period doubling. This is apparent from the notable difference of CF values given by CF_{T1-ADV} and CF_{T2-ADV}.

In case of CF_{T2-ADV} , the presented results show positive features as in case of p-2 orbit and from the comparison with CF_{Basic} (Fig. 9), it follows that the stabilization was reached very quickly and precisely.

CF Version	CF _{T1-ADV}	CF _{T2-ADV}
K	-0.4828	-0.4154
$F_{\rm max}$	0.1904	0.2808
R	0.4390	0.4969
CF Val.	241,1852	2.85 10 ⁻⁶
Avg. IStab	84	145

Table 5: Results for p-4 orbit, CF_{T1-ADV} and CF_{T2-ADV}



Fig. 9. Best solution: p-4 orbit, CF_{Basic}, SOMA ATAA, complex simulation with $0 < x_{initial} < 1$, 100 samples



Fig. 10. Best solution: p-4 orbit, CF_{TI-ADV} , SOMA ATA, complex simulation with $0 < x_{initial} < 1$, 100 samples



Fig. 11. Best solution: p-4 orbit, CF_{T2-ADV} , SOMA ATO, complex simulation with $\theta < x_{initial} < 1$, 100 samples

Investigation on results of chaos control

This section presents a accumulation of research (Senkerik et al. 2007) and the results presented here. Please refer to Table 6 for the comparison of average number of iterations required for stabilization, which was elaborated for five CFs and all desired UPOs. Here, a gradual decrease of average IStab value together with development and testing of complex targeting cost functions can be clearly seen.

Table 6: Comparison of results for five CFs

UPO	p-1	p-2	p-4
CF Basic	77	124	122
CF Targ1	49	113	121
CF Targ2	39	108	118
CF Targ1 Adv.	56	51	84
CF Targ2 Adv.	41	133	143

The first CF Basic gives satisfactory results and can be used wherever the good quality of stabilization is expected and the speed of stabilization and "universality of this solution" for wider range of initial conditions are not decisive.

In case of targeting cost functions, the results for p-1 orbit are significantly better, on the other hand the slightly better results for higher periodic orbits (p-2 and p-4) were achieved at the cost of arising of problem with worse performance of EAs and obtaining of solutions with only temporary stabilization or none at all. This negative phenomenon culminates in case of CF_{T1-ADV} where the very low avg. IStab values represents the solutions with rapid and only temporary stabilization.

Finally, CF_{T2-ADV} design suppress all mentioned problems and gives excellent performance from the point of view of quickness and quality of stabilization for any initial conditions.

CONCLUSION

The optimization of chaos control described here is relatively simple and easy to implement. Based on obtained results, it may be claimed that all simulations give satisfactory results and thus EAs are capable of solving this class of difficult problems and the quality of results does not depend only on the problem being solved but also on the proper definition of the CF.

From the optimization results it follows, that they are extremely sensitive to the construction of used CF and any small change in the design of CF can cause radical improvement of the system behavior (as in case of CF Targ2 Advanced), but of course, on the other hand can cause worsening of observed parameters and behavior of chaotic system as well.

All achieved results give the following piece of knowledge.

CF Targ1 advanced is the example of an upgraded CF Targ1 design, which brings the advantage of automatically computed *SC* value, for the purpose of improving the behavior of controlled chaotic system for wide range of initial conditions. The results were for the first view satisfactory, but two very momentous problems arose – period doubling and very poor performance of EAs. These problems uncovered hidden non-optimal structure of CF Targ1.

In the last proposal of CF Targ2, there were only slight changes in CF design, but from the presented results it can be seen, how such a small change can influence the performance of a controlled system, especially when it is an extremely sensitive chaotic system. CF Targ2 advanced gives excellent results for simulations with wide range of initial conditions and seem to be the choice for the task of finding of "universal and robust solution". The problems with poor EA performance and period doubling were mostly suppressed here. The only disadvantage of this proposal is the relatively big computational-time demands.

Finally, it is hard task to propose a CF, which gives excellent results, especially "universal results" suitable for simulation with wide range of initial conditions. As repeatedly mentioned, the chaotic systems are extremely sensitive to proper settings of control algorithm and of course they are very sensitive to even very tiny change in any parameter. This extreme sensitivity is transferred into complexity of CF surface thus it is also hard task for EAs to find good solution. It is also difficult to determine the conditions for optimizations and subsequent simulations.

Furthermore parameter settings for EA were based on heuristic approach; therefore there is also possibility for the future research. According to all results showed here it is planned that the main activities will be focused on testing of evolutionary deterministic chaos control in continuous-time and high-order systems and finally testing of evolutionary real-time chaos control.

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FRAMEWORK FOR A MULTI-LEVEL EVOLUTIONARY ALGORITHM FOR CONSTRUCTION OPTIMIZATION

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Evolutionary Construction. Optimization,

ABSTRACT

In large-scale non-linear construction optimization problems, the capability of an algorithm to find the optimal solution is usually limited by the inability to evaluate the effect of change in the value of each decision variable on the overall outcome of the objective function. Current optimization algorithms evaluate the quality of generated solutions based only on the value of fitness/objective function. As such, these algorithms are limited in their ability to robustly reach optimal solutions. This paper presents a framework for an innovative evolutionary algorithm that mimics the behavior of electrons moving through electric circuit branches with the least resistance. In the proposed algorithm, solutions are evaluated on two levels: a global level against the objective function; and a local level by evaluating the potential of the generated value for each decision variable. This paper presents (1) the philosophy behind this work; (2) the concept adopted in developing the algorithm; and (3) the basic steps of the algorithm. The new algorithm is expected to enhance the optimization of complex large-scale optimization problems.

Algorithms,

INTRODUCTION

Optimization plays an important role in enhancing the efficiency and ensuring the economic feasibility of various applied systems in the construction industry. Throughout the years, several optimization techniques, algorithms, and models were developed to deal with a multitude of problems within the industry. In the past, simple mathematical techniques were used to solve many simple optimization problems. With the technological advancement of computing systems and the need for powerful optimization techniques, several sophisticated optimization systems were developed to solve many complex problems that were hard to solve in a polynomial time frame (NP-hard). In 1975, John Holland developed genetic algorithms (GAs) simulating the Darwinian principle of evolution and the survival of the fittest (Goldberg 1989). Several other algorithms followed, modifying the original approach, in order to overcome the limitations demonstrated in the inability to reach optimum/near optimum solutions in reasonable time. In 1989, Pablo Moscato developed the memetic algorithm (MA) based also on the Darwinian principle of evolution, but his main contribution relied in adopting Dawkins' concept of a meme. Other EAs were also developed simulating various natural phenomena of biological evolution or social behavior of individuals. Example of these EAs are: particle swarm optimization (PSO), ant colony optimization (ACO), shuffled frog leaping (SFL), harmony search (HS) and others (Elbeltagi et al. 2005).

In the past decade, the application of evolutionary algorithms (EAs) in construction served as a quite acceptable alternative technique for solving complex optimization problems. Examples of EA applications appeared in various engineering disciplines (Feng et al.1997; Leu and Yang 1999; Haidar et al. 1999; Hegazy and Ersahin 2001; Hegazy and Wassed 2001; Lu 2002; Maier et al. 2003; Shyu et al. 2004; Solimanpur et al. 2004; Aguilar 2004; Christodoulou 2005; Elazouni and Metwally 2005; Elbeltagi et al. 2005; El-Rayes and Kandil 2005; Zehng et al. 2005; Khalafallah and El-Rayes 2006).

Most EAs are directed towards reaching optimality through the simulation of the behavior of certain species in certain ecological systems. The diversity in types of creatures that have evolved over the centuries makes the number and types of EAs simulating their behavior unlimited (Wu and Banzhaf 1998). In EAs, a pool of solutions (population) is created, where each individual in the population is modeled as an array. The merit of each array is evaluated with respect to an objective function throughout several cycles of evolution.

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PROBLEM DEFINITION AND STUDY OBJECTIVES

The developed EAs are considered in many cases computationally inefficient, especially in optimizing large-scale complex construction systems. In many of these complex optimization problems, it could take several days of parallel computing in order to reach a near optimal solution. This limitation could be attributed to two main factors.

First, EAs deal with candidate solutions indifferently and do not consider the potential of each individual solution. For instance, GAs simulate the behavior of human beings through its search for the best genes in a population of chromosomes representing a group of individuals. All genes constituting a chromosome receive same appreciation, when the fact is there are good and bad genes within the same chromosome. Although the processes of crossover and mutation may help in promoting some of the promising individuals and/or genes, chances of reaching the chromosome with the optimal solution is very limited. Another example is the individual ant in ACO, where each ant represents a solution string whose values receive the same pheromone reward regardless of the individual quality of the values in the solution string.

Second, current EAs strive to simulate the behavior of change without paying much attention to the change in the surrounding environment. Most species adapt to the changes in the ecological system surrounding them; and that is the main reason of their survival. They adapt by changing their behavior, while most EAs adopt the common behavior that is not necessarily guaranteed to be the best. This greatly affects the efficiency of the algorithm. For example, Dorigo's ACO is based on simulating the foraging behavior of ants and their ability to select the shortest paths between nests and sources of food. Deneubourg and collegues in 1989 and 1990 investigated the foraging behavior of ants through an experiment in which they utilized a double bridge to connect a source of food with a nest of ants of the Argentine type. They ran three experiments; in each one, they changed the lengths of the bridges. In one of the three experiments, the ants did not choose the shortest path (Dorigo, and Stutzle, 2004).

To overcome the shortcomings of other EAs, two points were taken in consideration. First was the quest for a natural phenomenon whose individuals' behavior is always consistent. Second, it was essential to find a way to evaluate the performance of the each entity in the system independently. This paper presents a framework for a new innovative multi-level evolutionary algorithm – under development – that tries to overcome the aforementioned limitations. The proposed algorithm is designed to mimic the behavior of electrons in a multi-branch electric circuit, where the majority of electrons join the branch with the least resistance. The following sections illustrate the methodology adopted for this study, the proposed multi-level evolutionary algorithm, and the planned future efforts to overcome the current algorithm limitations.

RESEARCH METHODOLOGY

The electric current is induced by the flow of electrons in a designated medium. The intensity of current induced is based on the resistance of the medium to the flow of electrons through it. Therefore, changing the medium's resistance will change the intensity of the current; i.e. number of electrons passing through it.

In the proposed algorithm, candidate solutions for the objective function are generated randomly. Each solution represents a wire with an unknown resistance. Each value in the solution string represents a segment in the wire of different material and different resistance connected in series as shown in Figure 1. Therefore, there is a global resistance for the whole wire (solution string) and a local resistance for each value comprising the solution.

The individuals of the population of solution strings (wires) are connected in parallel representing an electric circuit as shown in Figure 2. The electrons flow in the circuit due to a potential difference in a source whose voltage is selected based on the type of the problem. Each wire is evaluated globally with respect to all the other wires, and each segment in the wire is compared to other local segments within the same wire. The global and internal individual resistances are then computed for each wire and its segments, as described in more details in the following section. The whole circuit is then demolished, and a new circuit is constructed using the best wires identified in the previous cycle. The process is iterative till the wire with the best conductivity is created (i.e. optimum solution).

The basic difference between the proposed EA and other EAs relies in the evolution process. In traditional EAs, the species (solutions population) evolve and are ranked with respect to an objective function to tell how good they are until they reach superiority (optimum value).



Figure 1: Schematic Diagram of Solution Strings (wires)

On the other hand, in the new EA the electrons do not evolve, but their surrounding environment (electric circuit) does. The electrons are merely identical agents with consistent behavior; they select the path with the least resistivity and go through the electric circuit, telling how good the conditions are.



Figure 2: Solution Population Represented as an Electric Circuit

MULTI-LEVEL EVOLUTIONARY ALGORITHM FOR OPTIMIZATION

The proposed algorithm is iterative where a number of wires (solution strings) are created, tested, and readjusted. The basic steps of the algorithm are as follows:

- 1. Construction of trial solutions: This is done by fabricating a number of wires (*N*) composed of *n* segments of different material connected in serious. Each segment is randomly enumerated to represent a *resistance* value r_n in the solution space, as shown in Figure 1.
- 2. Construction of the electric circuit: Once all wires are fabricated, they are connected to an electric source of voltage *V*. The value of *V* is selected based on the type of problem, as shown in Figure 2.

- 3. Calculation of the current intensity *I*: For each wire, the intensity of current I_N passing through it is calculated. This is achieved by substituting the randomly selected value of each wire in the objective function.
- 4. Determining resistance of wires (R_N): The global resistance of each wire is calculated using *Ohm's Law:* $R_N = V/I_N$.
- 5. Quality of wires: This is determined by the relative importance Z of W_N compared to other wires in the solution space. The relative importance is based on the current intensity I_N according to equation (1).

Relative Importance (
$$\mathbf{Z}$$
) = $\frac{\mathbf{I}_{N}}{\sum_{l=1}^{N} \mathbf{I}_{N}}$ (1)

6. Quality of selected values: The quality of each value in W_n is determined by calculating its internal resistance r_n . At first, it is assumed that all resistances r_n for segments *n* appear identical since there is no prior information about how good the solution is. Therefore the resistances are calculated according to equation (2).

$$r_{nv} = \frac{R_N}{n} \tag{2}$$

In order to determine the actual resistance of each value, a sensitivity analysis is conducted by substituting the value v of each segment in a sample *S* of the wire population. The change Δr is then recorded and the resistance is calculated according to equation (3).

$$r_{\text{mod ified}} = r_{nv} - \sum_{1}^{S} (\Delta r_{nv} \times Z_{S})$$
(3)

Where r_{nv} = internal resistance of selected value v in the original wire W_n ; Δr_{nv} = difference between the original resistance and the new

resistance after substituting the value v in W_s ; S= sample size; Z_s = relative importance of the wire selected.

The calculated resistances r_n for different values v_n of the same wire W_n are then normalized with respect to the global resistance R_n . This guarantees that there is no violation to Kirchhoff's rule.

The sample size (S) can be determined using Cochran's equation (4).

$$\eta_0 = \frac{(t)^2 * (P)(q)}{(d)^2} \tag{4}$$

Where: η_0 = sample size; t = value selected for a designated alpha level; d = acceptable margin of error; and (p)(q) = variance in I_N .

7. Updating resistance (r_n) of selected values: the resistance r_n of selected values v is updated according to equation (5):

$$r_{\text{vupdated}} = \text{Min} \left[r_{\text{v}}(m-1), r_{\text{v}}(m) \right] + \frac{\text{Min} \left[r_{\text{v}}(m-1), r_{\text{v}}(m) \right]}{\text{Max} \left[(r_{\text{v}}(m-1), r_{\text{v}}(m) \right]}$$
(5)

Where $r_{vupdated}$ = updated resistance for value *v*; $r_v(m-1)$ = resistance of *v* at previous iteration (*m*-1); $r_v(m)$ = resistance of *v* at current iteration (*m*).

8. Selection of values: The selection process of values is based on the individual resistance associated with each value, which is updated after each iteration until the best conductor is created. The probability of selecting values for each parameter in the objective function is calculated according to equation (6).

$$P_{vn}(w_N, m) = \frac{1/r_{vn}}{\sum_{\nu} 1/r_{\nu n}}$$
(6)

Where P_{vn} = probability that value *v* is selected for segment *n* in wire W_N at iteration *m*; r_{vn} = resistance of value *v* selected for segment *n*.

It is worth mentioning that this method of selecting values guarantees the deployment of all values in the solution space at least once. This is due to the fact that the initial resistance r_n of all values at iteration (m=0) appear to be identical and have a value of 1.

The flow chart for the proposed algorithm is shown in Figure 3.

OBSERVATIONS AND FUTURE RESEARCH

During the development of the algorithm, several hardships were encountered. The main one relied in finding a suitable way to evaluate each value in the solution string independently.



Figure 3: Flowchart of the Proposed Algorithm

As mentioned earlier, each solution string is evaluated globally and locally. The basic idea for evaluating the performances of different values of variables of the objective function revolved around finding a suitable method to calculate the internal resistance of the wire segments. Several attempts were made to come up with a sound way to evaluate each value independently, i.e. calculate local resistance r_n .

The coefficients of the objective function variables were investigated to serve as a suitable measure for the performance of different values. In optimization, the coefficients of the objective function play a very important role in determining the optimal solution. For instance, in linear programming, changing the coefficient of the objective function changes the optimal solution. Consequently, the variable with the highest coefficient contributes the most in maximization problems (Winston, 1993). Hence, the basic idea was to initially assume that the local resistance r_n is a proportion of the global R_n with a value of [($C_n/\Sigma C_n$) x R_n], where C_n is the coefficients of variable *n*. However, this practice is not practical for all optimization problems. This is due to the fact that in most cases the solution string does not carry real values of the objective function variables. For example, consider the case study appeared in (Elbeltagi et al., 2005) for the time-cost tradeoff problem. The solution strings carried indices referring to various construction methods of different times and costs. This means that each single value is meaningless if plugged directly in the objective function.

A special attention was given to the signs of the coefficients of the objective function, and the type of connection between the wire segments. The segments of the same wire can be connected in series or parallel based on the sign of the coefficients. Consider the following hypothetical trivial objective function: [Maximize: 7a-3b+4c]. Since it is a maximization problem, the values for variable a and c should be as high as possible, and as low as possible for variable b. The ideal way to model this function, is to have the wire segments for variables a and c connected in series, and the segment for variable b connected to them in parallel as shown in Figure 4. However, in most cases and as mentioned earlier, the values of the solution strings do not relate directly to the variable of the objective function. The assumption used in this algorithm is that all segments of the same wire are connected in series. That assumption makes sense for two reasons. First, the series connection would represent the general case for all problem domains. Second, in real life, two points on an electrical circuit could be connected by two or more different wire segments joined in series rather than in parallel.

One of the basic advantages of this algorithm is its ability to evaluate each value of the solution string independently. The concept of the internal resistance of different segments within the same wire was found to be very convenient. This is due to the fact that the value of the internal resistance r_n is independent of the value of the objective function. In other words, the internal resistance is merely a measure of how good each value is. This guarantees no violation for Ohm's and Kirchhoff's rules as the only changing value is I_N .



Figure 4. Alternative Representation of the Solution String Based on the Signs of the Coefficients

A very interesting observation that is currently under investigation is the change in the potential of individual values for reaching optimal solution. Consider the electric circuit shown in Figure 5. The two wires are identical except for resistance r_1 . Table 1 summarizes the values of *I*, *V*, and *R*.



Hypothetical Optimization Problem

It can be noticed that when the value of resistance r_I changed in the second wire, the value of I across the wire was doubled, and the potential difference across the nodes of resistance b, and c was doubled though their resistance values did not change.

Table	l. Summary	of Values	of I, V,	and R	of the
	Cire	cuit in Fig	ure 5		

Wire	1	2
R(equiv.)	24 ohm	12 ohm
I	0.5 amp	1 amp
Va	8.5 volt	5 volt
Vb	1.5 volt	3 volt
Vc	2 volt	4 volt

It can be interpreted that the solution string represented by W_1 is a good candidate; however, a slight change in one of its values made it the best.

CONCLUSION

This paper aims to present the framework of a new evolutionary algorithm. The basic advantage of this algorithm lies in its multi-level evaluation process. Each value is evaluated twice. First, the selected value is evaluated globally by comparing it to the other values in the solution space. Second, the selected values are evaluated locally by comparing their relative potential in affecting the objective function. The paper presents a quick overview of the philosophy, concept and optimization steps for the proposed algorithm. The algorithm is planned to be tested on several optimization benchmarking problems to evaluate its efficiency.

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Agent-Based Simulation

SIMULATION OF AGENT TEAMS: APPLICATION OF A DOMAIN-INDEPENDENT FRAMEWORK TO COMPUTER NETWORK SECURITY

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Agent-based Simulation, Intelligent Agent Teams, Network Security, Distributed Denial of Service.

ABSTRACT

The paper proposes an approach for multi-agent simulation of intelligent agent teams' collaboration and competition. This approach is for representing the complex processes ongoing in different subject domains by using various types of agent teams and their interactions. Teams can be in relations of indifference, antagonistic and non-antagonistic competing or (and) various kinds of cooperation, and may adapt to the actions of opponents or collaborators. The domainindependent multi-agent framework and common simulation environment are proposed. The suggested approach differs from other related approaches by attempting to formalize main components needed for agent teamwork and team collaboration and competition. The approach is applicable for the tasks of competitive activity in commerce, counteraction in the Internet, simulation of rescue operations, coalition actions, military conflicts, etc. We consider the theoretical models, implementation and investigations of the proposed approach on an example of simulation of distributed Internet attacks and defense.

1. INTRODUCTION

Due to a set of reasons the distributed complex systems cannot be automated effectively on the basis of traditional architectures, methods and software tools. These systems demand the possibility of implementing the dynamic behavior, autonomy and adaptation, using the methods based on negotiations and cooperation that lie in the basis of agent-oriented systems. The effective implementation of these systems requires thorough and comprehensive simulation.

There was developed the variety of frameworks and architectures for multi-agent simulation of distributed complex systems, e.g. shared plans theory (Grosz and Kraus 1996), joint intentions theory (Cohen and Levesque 1991), hybrid approach (Tambe 1997), there were implemented various software multi-agent environments (Macal and North 2005; Marietto et al. 2002). The approaches based on belief-desire-intention (BDI), distributed constraint optimization (DCOP), distributed POMDPs, and auctions or game-theoretic (Tambe et al. 2005) are emphasized. Different mechanisms for collaborative agent team maintenance are suggested (Kaminka et al. 2007). The main task of these approaches is to provide the optimal interaction of heterogeneous components (including robots, smart devices, machines, software agents and people) to reach some high level goal. These methods, models and tools have been applied in different subject domains (Haque et al. 2005; Jennings 1995; Kaminka and Frenkel 2005; Tambe 1997; etc.). But the approaches mentioned lack the detailed description of the aspects needed for simulation of competing agent teams. There are several multi-agent simulation system implementations for imitating antagonistic opponents. For example, Robocup Soccer implementations use mainly reactive agents, TacAir-Soar simulates combat pilots, there is a network intrusion simulation implementation for MASON simulation toolkit (Luke et al. 2004), etc.

The paper proposes an *approach that allows to simulate* and investigate the work of collaborating and competing agent teams. We examine the interaction of at least two agents teams that can be in the relation of antagonistic and non-antagonistic competing or (and) various kinds of cooperation, and may adapt to the actions of opponents or collaborators. The approach suggested in the paper differs from other related approaches by (1) attempting to formalize main components needed for agent teamwork and team collaboration and competition, (2) emphasizing various types of interactions between agent teams and (3) developing the multi-level simulation environment that allows to use as the basis the various discrete-event simulators and the libraries (ontologies) of different subject domains. The global goal of our research is to develop domain-independent framework and common simulation environment (integrated software tool) for analysis of intelligent agent teams as well as to implement them for investigation of several important application domains: simulation of rescue operations, simulations of social-technical networks, simulation of Internet attacks and defense, etc.

The paper is organized as follows. *Section 2* outlines the proposed approach to the simulation of competing agent teams. *Section 3* describes the architecture of proposed simulation environment. *Section 4* considers

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several important domains which require the investigation of competing agent teams' behavior. *Section 5* examines the application of proposed for the multi-agent simulation approach of counteraction of malefactors and defense systems in the Internet. Section 6 represents the conducted experiments. Conclusion surveys work results and future research.

2. SIMULATION FRAMEWORK

The proposed approach supposes that counteraction, competition or cooperation in a particular system (subject domain) is represented as the interaction of various teams of software agents. The aggregated behavior of this system is revealed due to local interactions of particular agents in the dynamic environment defined by the agent interaction model. Classes of agent teams are selected depending on the solved task and subject domain. For example, for some tasks of information counteraction one can use at least the following three classes of agent teams according to the realized strategy: the class of attack teams; the class of defense teams; the class of agents imitating some background processes. In this case the goal of attack team is to detect the vulnerabilities of the environment and defense system and to realize the given list of threats due to executing the attack actions. The goal of defense team is to protect the environment and its own components from these actions. Agents of different teams compete to reach the opposite goals, collaborate to fulfill the attack or defense task or are in an indifference relation. Agents of the same team collaborate to reach the joint intention (to realize the threat or to defense the environment).

The developed domain-independent multi-agent framework for simulation of agent competing includes the following components: (1) The ontology of application domain containing application notions and relations between them (we differentiate the problem ontology, the shared application ontology, the application ontology of particular team and particular agent); (2) The protocols of teamwork for the agents of different teams; (3) The models of scenario behavior of agents for team, group and individual levels; (4) The libraries of agent basic functions; (5) The communication platform and components for agent message exchange; (6) The models of functioning environment, including topological, functional and other components; (7) The models that provide the interaction of teams (antagonistic and non-antagonistic competing or various kinds of cooperation). The approach for teamwork is based on combining the elements of joint intentions theory, shared plans theory and combined approach. The mechanisms of agent interaction and coordination are based on the procedures of action consistency maintenance, monitoring and agent functionality recovery, and communication selectivity (Tambe 1997).

The following main simulation components are represented on the basis of this approach: models of agent teams; models of team interactions; interaction environment model. Models of agent teams are intended for the representation of investigated processes. They include particular team ontologies, agent basic functions, agent classes, agent protocols, behaviour scenarios. Team ontologies are based on the subject domain ontology and include the notions and relations used by agents of this team. The list of agent basic following functions includes the functions: initialization; shutdown; access to the agent ontology; management of active agents list; basic work with transport-level modules (connection establishing, message sending, connection closing). The needed agent classes are defined for the teams. The amount of agents of predefined classes is set in each team. Agent interaction protocols are represented as the sequence of instructions with specific parameters. The type of instruction defines how to use these parameters. The conditions of protocol initialization provide communication selectivity for agents. Agent interaction protocols are based on the transport layer that is provided by the communication environment. For example, the developed protocol for agent team establishing is based on dividing agents into "clients" and "servers". The first send the messages about their existence to "server". Server contains the list of agents in the team. Periodically it checks the agents in this list to actualize it and to know which of agents are active. Agent team establishing protocol is the part of procedures for monitoring and recovery of agent functionality. Scenarios represent various stages of team actions. Adaptation procedures are implemented in scenarios to act depending on other team actions and environment reaction. Agent teams' behavior scenarios ensure action consistency maintenance. Models of team interactions include the models of antagonistic competing, team cooperation and adaptation. Model of antagonistic competing lies in the basis of competing teams' interaction. This model defines the goals, subgoals, intentions and actions of competing teams that are aimed on the interaction environment or (and) the opponent team. Cooperative interaction happens between teams that pursue the same goal. The proposed model of cooperation is based on the exchange of information between teams. Such exchange is made to raise the effectiveness of reaching the common goal and occurs on several different levels with the use of agents of various classes. For example, in the task of cooperative network defense simulation it is possible to exchange attack signatures, network traffic data, filtering requests, etc.

Adaptation is in reacting to the actions of other teams and environment changes by modifying the scenarios of team behavior. Adaptation model of agent team T_1 according to the actions of competing team T_2 and environment changes is in the following. When the efficiency (or severity) S(t) of team T_2 actions and (or) the interaction environment changes, then such configurations and scenarios K(t) of team T_1 behavior are chosen, that ensure the reaching of the given goal with minimization of sum of action cost functions C_i , i=1,...,n (n – number of main agent team goals):

$$F = \sum_{i=1}^{n} C_i(S(t), K(t)).$$
 (1)

Model of environment for agent teams' interaction allows determining such interaction environments that are characterized by various representation granularity that depends on the requirements for simulation fidelity and scalability.

3. SIMULATION ENVIRONMENT

To implement the proposed approach the special simulation environment (tool) was developed. To implement the approach the multilevel architecture of simulation environment was proposed. It consists of the following layers (Figure 1). Simulation Framework is supposed to be discrete-event simulator. Other simulation environment components are Simulation Framework modules and models. It can use for its functioning the various domain-oriented discrete-event simulation software tools and software libraries (Network Simulators; Simulation frameworks; Simtools; etc.). Environment Simulation Framework is a suite of simulation modules that allows to imitate realistically the environment for agent interaction. This component implements the communication environment and transport protocols models. Multi-agent simulation is realized due to Agent-based Framework that uses Subject Domain Library. The framework is the modules library that defines intelligent agents implemented as applications. FIPA (FIPA) abstract architecture elements are used during agent modules design and implementation. Agent communication language is used to allow the agents interact with each other. The messages between agents are transmitted on the top of transport protocol that is implemented in Environment Simulation Framework. Agent directory is obligatory only for the agent that coordinates the actions of other teammates. Agents are able to control other modules due to messages. Subject Domain Library (ontology) is the library that contains modules for imitation of subject domain processes. The libraries for different domains are supposed to be implemented and used.

The parameters of agent teams, their interaction and interaction environment are used as the input for the simulation tool. Simulation of the studied processes is made on the basis of the mentioned models. Simulation tool outputs the set of various parameters using which one can analyze the simulated system. Simulation process is defined due to the technique that includes various stages for parameters' input and processing, simulation of agent teams' behavior, parameters output and analysis.



Figure 1. Simulation environment (tool) architecture

4. EXAMPLES OF APPLICATIONS

We are intending to investigate the application of the agent-based framework and software environment for simulation of agent teams in several important domains and develop application-dependent models and software tools. Below three different applications are considered which are under investigation.

Simulation of rescue operations. In RoboCup Rescue, agents work in the virtual city. For example, agent teams can include a human fire chief and a number of robot or agent-controlled and managed fire brigades. The human fire chief is given a high-level view of the fire-fighting progress and can make better roleallocation decisions to save trapped and injured civilians and limit damage. The tasks are to rescue the civilians, buildings which are on fire and roads that are blocked. The problem is then how to assign ambulance teams, fire brigades and police forces to these tasks. We propose to represent several rescuers (e.g. fire brigades, ambulance and police) as an agent teams. These teams pursue the same goal and are able to cooperate and to adapt to each other actions. The cooperation is in asking the other team for the corresponding agent for help, e.g. when additional fire brigade is needed. Each rescue team adapt to the actions of another team by monitoring the current rescue operation and if the other team manages the situation than the first team switches to another operation. There can be existed additional teams representing the opposite site: the terrorists that are the reason of rescuing operations. They try to act in such a way that rescue operations will fail or be ineffective. This can be done to simulate the "worse case scenario". Also it is very important to simulate the ordinary people actions. They can be represented as a team of agents that needed to be rescued if they are injured.

Simulations of social-technical networks. There can be a lot of applications of the proposed approach in social networks (Rosvall Sneppen 2008). For example, stock market game, epidemic propagation, rumor spreading, etc. The proposed approach can be widened to represent a big variety of social relations and interactions based on them (excluding the already stated indifference, counteraction, cooperation and adaptation): values, ideas, financial exchange, friends, kinship, dislike, trade, web links, disease transmission (epidemiology), etc. These new interaction types also might be used to simulate other subject domains with higher fidelity. Simulating the antiterrorism actions is the most natural usage of the approach proposed. The simulated "terrorists - antiterrorists" processes are represented as counteracting teams of agents. They have the opposite goals. The teams from the same site cooperate and adapt to each other and opponents' actions. There is an important issue of cooperation between heterogeneous agents as humans and machines, or e.g. human squad and helicopter squad. It is proposed to create models of interaction on the different layers. Simulation of the competing companies is one of the other important applications. These companies are represented as the teams of competing agents. They interact not only on the basis of competing, cooperation and adaptation. There are financial exchange, trade and other types of interactions that have to be specified.

Simulation of distributed Internet attacks and defense. The investigation of counteraction of malefactors and defense systems in the Internet is one of the important tasks that have to be solved for designing the secure distributed computer systems. The design and implementation of effective cyber-defense intelligent cyber-defense system is a very complicated problem. According to our view the prospective network cyber-defense system has to be *fully integrated* and multi-echeloned one. To effectively detect the computer attacks or unauthorized operations and to flexibly react on them, it is needed to carry out the continuous control of network functioning, analyze possible risks, collect knowledge about counteraction, detection and reaction methods and use them for defense reinforcement. Besides, the effective cyberdefense should include the mechanisms of attack prevention, detection, source tracing and protection as well as can only be achieved by the cooperation of different distributed components which can be represented as different agent teams. This approach was implemented for the investigation of distributed denial of service attacks and defense mechanisms (Kotenko and Ulanov 2006; Kotenko and Ulanov 2007). Let us consider the last application domain in more details.

5. COMPETING AGENTS IN INTERNET

The investigation of counteraction of malefactors and defense systems in the Internet is one of the important tasks that have to be solved for designing the secure distributed computer systems. The representation of malefactors and defense systems as intelligent attack and defense agent teams are a very prominent idea. It is very topical in viewing the current tendencies in malware technologies which will emerge from the combination of classic network worms and viruses, distributed denial of service (DDoS) tools, root and kernel kits, botnets as well as concepts from network and artificial intelligence research, including peer-topeer (P2P) communications and intelligent agents. In the Internet security context, the defense of traffic that is generated by the agents-users is one of the important tasks for the defense agent teams. This is vital, for example, during counteracting the teams of agentmalefactors that realize DDoS attacks.

Traditional defense from DDoS includes detection and reaction mechanisms. To detect abnormal network characteristics, many methods can be applied (for instance, statistical, cumulative sum, pattern matching, etc). The examples of detection methods are Hop counts Filtering (HCF), Source IP address monitoring (SIPM), Bit per Second (BPS), etc. As a rule, the reaction mechanisms include filtering, congestion control and traceback. As detection of DDoS is most accurate when it is close to the victim hosts and separation of legitimate is most successful close to the sources. adequate victim protection to constrain attack traffic can only be achieved by cooperation of different distributed components (Mirkovic et al. 2005). There are a lot of architectures for distributed cooperative defense mechanisms, e.g. Server Roaming, Market-based Service Quality Differentiation (MbSQD) (Mankins et al. 2001), Transport-aware IP router architecture (tIP) (Wang and Shin 2003), Secure Overlay Services (SOS) (Keromytis et al. 2003), ACC pushback, COSSACK (Papadopoulos et al. 2003), Perimeter-based DDoS defense (Chen and Song 2005), DefCOM (Mirkovic et al. 2005), Gateway-based (Xuan et al. 2002). During DDoS attack and defense counteraction, the agent teams realize distributed action scenarios and adapt to each other actions. To realize DDoS attack, malefactors have to do the following: compromise a lot of hosts, deploy on them attack agents and then make a simultaneous attack on victim hosts or the entire Internet subnets. In turn, defense agents that try to block the traffic generated by the attack agents have to provide normal traffic transmission. The team of agents-malefactors evolves due to generating new attack types and instances, and the scenarios of their realization to overcome the defense. The team of defense agents adapts to the malefactors actions due to changing the security policy, choosing, creating and using new instances of defense mechanisms and profiles.

The proposed simulation approach was implemented to investigate the behavior of attack and security agent teams. The developed *attack team ontology* includes the notions and relations of subject domain "DDoS attacks". Attack team model contains two agent classes:

"daemon" executing attacks and "master" coordinating other attack agents. Attack team uses the following protocols: team establishing; workability check; attack parameters transferring; attack realization. The scenarios developed define the attack agent team sequence of actions. The defense team ontology includes the notions and relations of subject domain "Defense mechanisms against DDoS". The following classes of defense agents are proposed: initial data processing ("sampler"); attack detection ("detector"); traffic filtering ("filter"); traffic limiting ("limiter"); agent of investigation. Defense team uses the following protocols: team establishing; sampler data collection; sending the addresses of possible attack sources; attack agents defeating, etc. Scenarios define team's action sequences. The agents "limiter" apply various modes. The following mechanisms are used by detector: Hop Count Filtering (HCF), Source IP Address Monitoring (SIPM), Bit Per Second Filtering (BPS).

The model of antagonistic counteraction of attack and defense agents defines the following aspects of attack realization. Attack team during attack influences on the network and attack target and this impact is transmitted to the defense team via the network. Defense team during attack detection tries to apply some defined defense countermeasures due to the mechanisms: traffic limiting, traffic filtering and attack agents defeating. Defense team influences on the network by traffic limiting and filtering. It influences on attack team also: particular agents might fail to receive attack commands and the attack packets might be filtered also. Trying to defeat attack agents the defense team influence on them directly.

Cooperative interaction happens between teams that aim the common goal to defend or to attack the network. Defense teams exchange information to raise the effectiveness of attack counteraction, and attack teams do the same to make the attack more effective. The following four agent classes are used in the proposed approach for cooperation: samplers, detectors, filters and agents of investigation. Defense teams can interact due to various cooperation schemas: no cooperation - all teams work on their own; filter-level cooperation – defense teams can apply filtering rules on the other teams filters; sampler-level cooperation defense teams can receive traffic data from the other teams samplers; weak cooperation – defense teams can use some filters and samplers from other teams; full cooperation - defense teams can cooperate using all available data and filtering rules.

According to the proposed *adaptation model (see formula (1))*, when attack traffic volume S(t) changes the defense team chooses such team configuration and behavior $K_D(t)$ that minimize the amount of false positives $C_{FP}(S(t), K_D(t))$, false negatives $C_{FN}(S(t), K_D(t))$ and attack duration $C_T(S(t), K_D(t))$:

 $\min_{S(t)} \left[C_{FP}(S(t), K_D(t)) + C_{FN}(S(t), K_D(t)) + C_T(S(t), K_D(t)) \right].$

From the other side, when defense efficacy E(t) changes then the attack team chooses such team configuration and behavior that minimize the amount of packet sent $C_P(E(t), K_A(t))$ and the amount of daemons defeated $C_D(E(t), K_A(t))$:

$$\min_{E(t)} \left[C_P(E(t), K_A(t)) + C_D(E(t), K_A(t)) \right].$$

The model of computer network is defined as $Network = \{Tp, P, Tr\}$, where Tp – network topology; P – protocols; Tr – traffic.

The proposed integrated *simulation environment (tool)* architecture was implemented using OMNeT++ INET Framework and software modules implemented in C++. It was intended for multi-agent simulation of DDoS attack and defense mechanisms. There are used the following *specification elements to define the network models, attack and defense mechanisms*:

- *Network topology:* quantity and types of hosts, channels between them and their types. The possibility to deploy certain type of application (or agent) depends on host type.
- *Defense team parameters:* quantity of daemons; master's address and port used for interactions; daemon's port used to send attack packets; victim's address and port; time of attack; attack intensity; address spoofing technique.
- *Attack realization parameters:* victim type (application, host or network; one must define the IP-address and port of victim); type of attack (brute force (UDP/ICMP flood, smurf/fraggle, etc.) or semantic (TCP SYN, incorrect packets, hard requests, etc.)); attack rate dynamics (can be constant or variable); adaptation scheme, etc.
- *Defense team parameters:* address of defended host; detector's address and port for interactions; server's reply size and delay time; adaptation scheme (changing of defense mechanisms) depending on attack severity, etc.
- *Defense mechanisms parameters*: deployment location (source, intermediate or defended subnets); the stages the defense method can implement (attack prevention, attack detection, tracing the attack source, attack counteraction); detection technique (misuse and anomaly detection; one chooses one particular method or the set of methods), etc.
- User team parameters: quantity of users; server's address and port; time to start; quantity of requests to server, interval between them and their size; interval between connections.
- *Defense team cooperation parameters:* scheme of cooperation.
- *Simulation parameters:* simulation duration; quantity of experiments; initialization of random number generator.

6. EXPERIMENTS

Various experiments were conducted to analyze the possible actions and scenarios of agent teams as well as the applicability and efficacy of the framework and simulation environment developed.

Experiments for investigating the cooperative work of defense teams included simulation of the following mechanisms: DefCOM (Mirkovic et al. 2005), COSSACK (Papadopoulos et al. 2003), "no cooperation", "filter-level", "sampler-level", "full cooperation". The following agent classes are proposed to introduce in compliance with *DefCOM* architecture: "Alert generator" - detects an attack and warns about it other hosts in the DefCOM network; attack is detected if the traffic exceeds some threshold; "Rate limiter" limits the traffic that is destined to the attack target; "Classifier" - provides selective traffic limiting, tries to classify attack and legitimate packets and to drop the former. COSSACK architecture consists of the following agent classes: "snort" prepares the statistics on the transmitted packets for different traffic flows; the flows are grouped by the address prefix. If one of the flows exceeds the given threshold then its signature is transmitted to "watchdog"; "watchdog" receives traffic data from "snort" and applies the filtering rules on the routers. Agent "snort" is based on the agent "sampler", and agent "watchdog" - on the agent "detector". HCF, SIPM and BPS local defense methods were used. Network topology was defined using the power function of frequency distribution of data links and hosts number was 50. For client team the defended server, 10 clients and their requests parameters were defined. Attack team included 10 daemons that realize UDP flood attack on server. Four defense teams are configured in compliance with the mentioned cooperative defense schemas. Conducted experiments showed the effectiveness of various cooperation schemas of defense teams. Attack traffic was sufficiently lowered regarding the start of attack. The best cooperative schema on the basis of output parameters is "full cooperation" (Figure 2, attack traffic is lowest after 450 s). Samplers-agents cooperation played the crucial role in defense.

Different *adaptation schemas of agent teams* were studied. *Adaptation schemes* operate in the following way. Depending on attack state the defense team adapts the parameters of methods and cooperation reducing the defense cost. The most simple and not resource-intensive method is BPS. Defense team starts the defense implementing BPS. When attack is detected the team continues to use the same method, if it allows to neutralize the attack. If it fails, then defense team applies more complicated SIPM method. If it succeeds to stop the attack, then the defense team returns to BPS. If not - it will additionally use HCF. Conducted experiments showed that one can reach the best attack traffic blocking due to defense teams cooperation.



Figure 2. Dependences of attack traffic volume on time for different cooperative schemas

Since sampler cooperation was the determinative in defense it can be used without applying full cooperation during which high teams interaction traffic is observed.

Attack team redistributes the attack intensity between daemons and changes the address spoofing technique to minimize the amount of attack packets and reduce the probability of attack agents' exposure by defense agents. At first the team having many daemons distributes the load equal between them and does not use address spoofing (not to draw suspicion upon themselves from firewall in their subnet). If after the defense team actions some of the daemons will be defeated, the attack team will raise the load to the remaining daemons (to save the given attack intensity) and apply address spoofing technique to avoid detection. If the remaining daemons will not be defeated the team will continue the attack in former mode.

Adaptation schema is tested in various cooperation modes (Figure 3). Cooperative team learning is supposed in sampler-level and full cooperation.



Figure 3. Dependences of attack traffic volume on time using adaptation criteria

7. CONCLUSION

The paper proposed a framework *for multi-agent simulation* of competing teams of intelligent agents. The framework is characterized by attempting to formalize all components needed for supporting agent teamwork and team competing. The *simulation environment* implementing this framework was developed. It is a multi-level software tool which allows to use the various discrete-event simulators and the libraries (ontologies) of different subject domains. The proposed approach was implemented on an example of multiagent simulation of the Internet attacks and defense mechanisms. The attack and defense teams' competing was implemented. The experiments showed the applicability and efficacy of the framework and simulation environment developed.

Future work is concerned with further formalization of antagonistic and non-antagonistic competing as well as various cooperation schemas of agent teams. Other direction of research is improving the simulation environment. We are supposed to develop and implement improved adaptation and self-learning mechanisms (as the current are prone to manipulation by opponents). The investigation of other applications for the framework suggested and the environment implemented (together with expansion of subject domain library) is very important. The essential part of future research is providing numerous experiments to analyze the framework and simulation environment.

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BIOGRAPHY



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AVOIDANCE OF NORM VIOLATION IN MULTI-AGENT ORGANIZATIONS

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KEYWORDS

Multi-agent organization modeling, norm violation, avoidance

ABSTRACT

In contemporary society not adhering to norms is something which is unwanted. Currently approaches to prevent this from happening are often taken whereby the deviation of a norm is punished and possible repair actions are performed. However, this is a reactive approach and can only happen once the norm has already been violated. This paper presents a proactive approach which allows intervention before the deviation actually occurs. In order to do this, an approach is specified for agents that enforce norms and can influence the input states of agents. This approach includes learning of input/output correlations of these agents by constructing decision trees, and utilizing this decision tree to intervene such that norm violation can be avoided. The approach is evaluated in the domain of Criminology.

INTRODUCTION

In order for agent societies to function in an effective and structured way, the paradigm of multi-agent organizations and institutions is a perspective which has been used by a variety of authors (see e.g. Ferber and Gutknecht 1998; Hannoun et al 2000). In such approaches, societies are specified by means of a structure (for instance by means of roles), as well as the expected behavior of such an organization. Norms (see e.g. Castelfranchi 2000) can be used to specify this expected behavior. A crucial point of specifying this behavior is that the agents participating in the society comply with these norms, as violation of these norms can potentially be harmful for the society as a whole. Hereby, several approaches have been developed to detect and punish these violations by using enforcer agents, possibly repairing the consequences (see e.g. Vazquez-Salceda et al 2004; Boella and Van der Torre 2008).

When looking at human societies a variety of organizations is present that enforce norms and punish those who violate the norms e.g. the judicature and the

police. These efforts are however not limited to punishing the society members that have already violated the norms, but also efforts are performed to avoid these violations.

This paper uses the idea to prevent norm violations from human society, and translates it to the domain of normative organizations. The approach is intended to support humans in preventing norm violation by being advised by an agent, or by letting the agent itself proactively intervene. The approach itself is presented in a highly generic format in order to make it reusable. Such a generic approach is however difficult to evaluate. In this paper an evaluation has therefore been conducted within a specific domain, namely Criminology, because this is a typical area in which norms are frequently violated. Criminology is a social scientific area which focuses on all aspects of criminal behavior. So on prevention as well as on punishment, making it very suitable as an application domain.

The approach is developed under the assumption that these advisory or norm avoidance agents can observe the input and output states of other agents participating in society and influence particular input states of agents. Ideally, these agents would simply avoid unwanted actions from occurring, but these might not all be controllable. Therefore, in the approach first of all algorithms are present for learning the input/output correlations of the agents in the society. This can be learned by either taking an external perspective, not knowing the internal functioning of an agent, or by having full knowledge of the internal functioning of this agent. This correlation can be used to predict whether the current input states of the agent lead to an unwanted output state. In case norm violation is predicted using these correlations, methods are introduced to avoid this violation from occurring by influencing the input states of the agent.

The paper is organized as follows. First, generic formalisms to avoid norm violation are presented in three parts: (1) a part that enables derivation of norm violation and representation of input and output states of an agent; (2) the learning of input/output correlations of agents, and (3) methods to avoid norm violation. Thereafter, the approach is thoroughly evaluated for a case within the domain of Criminology to see how well the system would function in such a domain. Finally, a discussion is presented.

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AGENTS AND NORM VIOLATION

This section discusses the perspective taken towards agents within a particular organization, and the norms that are specified to constrain the behavior of such agents. Note that the formalisms introduced here for agents and norm violation are meant as a way to specify the approach to prevent violation of norms, the idea is therefore to introduce a very simple notation to allow a clear explanation of the approach. Of course, much more advanced formalisms can be used as well, but that is not the aim of this paper.

Viewpoint Towards Agents

The *external viewpoint* towards agents is represented by means of input and output states of the agent. An input of an agent a can be built up using elements from the set of possible *observations* the agent can receive, expressed by the ontology $O_{in(a)}$. In addition, an input state of an agent can consist of *communication*. Hereby the ontology of communications an agent can receive is represented in the set $C_{in(a)}$. Output states of an agent can include *communication* ($C_{out(a)}$) or *actions* ($A_{out(a)}$). Together these sets form the ontology for external states:

 $Ont(a) = O_{in(a)} \cup C_{in(a)} \cup C_{out(a)} \cup A_{out(a)}$

In order to derive what is true in the world, truth values are assigned to each of the atoms that can be created using the set Ont(a). This combination is referred to as the set Ext(a), with which the actual occurrence of external states of the agent can be described. The occurrence of the truth values of these elements varies over time. The dependencies between elements are represented in temporal logic. Furthermore, it is assumed that a *history* of the agent can be maintained by storing previous states of the agent. Hereby a previous state is made explicit by means of the prev predicate (which can be nested up to s states back in time), which can be built as follows:

 $PrevState(a) = prev^{n}(Ext(a)) \text{ where } 1 \leq n \leq s \text{ and }$

prev¹(Ext(a)) = prev(Ext(a))

Besides an external viewpoint towards an agent, more might be known about the *internal processes* of the agent as well. Hereby, internal states can become necessary, for example beliefs, desires and intentions (e.g. Rao and Georgeff, 1991). These states can be expressed in a similar fashion as the input and output. Dependencies between the different states can be represented by using a temporal logic. For example, an observation o_1 can lead to an action a_1 being performed in the next state, in case this is true, this can be specified in temporal logic as follows: o_1 , $\rightarrow o a_1$

Norm Violation

As already argued in the introduction, violation of norms by agents is unwanted. Several mechanisms for detection of norm violation have been proposed (see e.g. Boella and Van der Torre 2008). The assumption in this paper is that given a set of external agent states it can be determined whether a norm is violated. The focus is on the single agent case, therefore, the norms addressed do not concern multiple agents. Assume a certain norm n_1 from the set of norms for an agent a called N_a (i.e. $n_1 \in N_a$). A subset of the current inputs and outputs of the agent and the input and outputs that occurred in the past can determine whether such a norm will be violated at some point in time in the future (i.e. the norm does not hold at that time point):

NormViolationSt(a, n_a) $\rightarrow \Diamond \neg n_a$

where NormViolationSt(a, n_a) \subseteq (Ext (a) \cup PrevState(a)) Hereby, the condition is that this set is minimal:

–∃NormViolationSt2(a, n_a):

NormViolationSt2(a, n_a) $\rightarrow \Diamond \neg n_a \land$

NormViolationSt2(a, n_a) \subset NormViolationSt(a, n_a)

For instance, if the norm n_1 states that action a_1 should never be performed, the fact that the agent performs the action makes that this norm is violated: $a_1 \rightarrow 0 \neg n_1$

IDENTIFYING POTENTIAL NORM VIOLATION

This section addresses how potential violation of norms can be detected, for instance by an advisory agent for a human. Hereby, a distinction is made between the case whereby a complete internal model of the agent is present, and the case whereby only an externally observable history of the agent is present (i.e. the input and output states).

Externally Observable History

In order to identify the states of the agent that lead to the occurrence of a norm violation state, it is assumed that the advisor agent can observe the external states of an agent at all times. See the last section for a brief discussion on this assumption. In order to learn the correlation that exists between the occurrence of these external states and the set which implies violation of a norm, a data mining algorithm is used. More in specific, the ID3 algorithm as proposed by Quinlan (1979). This algorithm can be used to construct a decision tree based upon which it can be determined whether the recent history and present states of the agent imply the future occurrence of the norm violating set.

The algorithm works as follows: an attribute (in this case the attributes are states of the agent) is chosen which minimizes the function that calculates the information entropy:

$$E(A) = -\sum_{i=1}^{V} \frac{S_i}{S} \sum_{j=1}^{N} \frac{k_{ji}}{S_i} \log_2 \frac{k_{ji}}{S_i}$$

Whereby V is the number of values for attribute A, (in this case 2, true and false), S is the total number of examples, and S_i is the total number of examples where A has the ith value. In this specific case, the examples concern the input and output states of the agent that are not present within the NormViolationSt(a, n_a) set, and the occurrence of the specific set NormViolationSt(a, n_a) which is the classification of the examples (i.e. whether the norm will be violated or not). Furthermore, the history which is taken into consideration is limited (it is not the

aim to take the complete history into account). Therefore, the number of previous states is limited to δ :

IndicationViolation(a, $n_a) \subseteq$

(Ext (a) \cup prev(Ext(a) $\cup \dots \cup$ prev[§](Ext(a))) where IndicationViolation(a, n_a) \cap NormViolationSt(a, n_a) = \emptyset

N in the equation to calculate the entropy is the number of categories for the classification. In this case, it is always equal to 2 since a norm violation state can occur or not. Finally, k_{ji} is the number of examples in the jth category of the classification that have the ith attribute value. Given that such an attribute is chosen based upon this function, the examples are partitioned according to the attribute values of the chosen attribute. This process is continued iteratively, unless the set of examples consists of merely one category for classification. Then the leaf is simply labeled with that category. In addition, several mechanisms can be used to avoid overfitting the data, such as *chi-squared* pruning (Quinlan 1979).

Imagine the very simple scenario whereby the set NormViolationSt(a, n_1) consists of one element, namely a_1 , and a_1 is observed to be the case in the current state. Furthermore, the only relevant history is the previous state, in which o_1 was true. Then, the following input will be presented to the ID3 algorithm (the states are in the top row of the table and the accompanying truth values in the second row):

prev(o1)	NormViolationSt(a, n1)
true	true

The resulting decision tree will be trivial in this case, namely just 'true'.

Complete Internal Model

In case a complete internal model is present of the agent (this is for instance common in Criminology in case a detailed psychiatric report is present), a decision tree can be constructed as well based upon the external states. The underlying assumption is that the values of the internal states of the agent that do not depend upon external states are known, and do not change over time. The external states considered in the decision tree are the current states, and the history up till δ steps back. This set is defined as follows:

$$\label{eq:relation} \begin{split} \text{RelevantStates}(a) &= \text{Ext}~(a) \cup \text{prev}(\text{Ext}(a) \cup \cup \\ & \text{prev}^{\delta}(\text{Ext}(a)) \end{split}$$

Given this set, a decision tree can now be constructed to indicate a certain norm violation set NormViolationSt(a, n_a) occurring as specified in algorithm 1 below. Note that the algorithms are not presented in a full formal format for the sake of clarity.

Algorithm 1. Constructing Decision Tree using Internal Model

Start by constructing a root node of the tree which represents the state without the truth value in the first element in the set RelevantStates(a). Construct two branches labeled true and false. Set i=2

 if i ≤ |RelevantStates(a)| For each branch without a node attached: construct a node labeled with the state without the truth value of the ith element in RelevantStates(a). Construct two branches labeled true and false for each of these nodes, and set i = i + 1 and return to 1.

- else use the ontological elements and the truth values from the path from source to this leaf, and the internal model (including the values of states that are not dependent upon external states) to determine (by means of inference) whether these values result in at least one possible state that indicates the violation of a norm (i.e. NormViolationSt(a, n_a)) holds).
 - if this is true, set this leaf to NormViolationSt(a, $\ensuremath{n_a}\xspace)$ being true

else set NormViolationSt(a, na) to false

As a result, a decision tree consisting of all (external) states, and a partial history, is constructed by means of which it can be determined whether a norm will be violated.

AVOIDANCE OF NORM VIOLATION

Given that it can now be predicted whether a norm will be violated, preventing this norm from being violated is the next step. In order to achieve this, the advisor agent needs advise the human how to change the world states to alter the input states of an agent (or proactively perform the changes itself). Since both the internal as well as the external norm violation model result in a decision tree, such a tree is taken as a basis. In this step, it is assumed that the violation of a norm is always more costly than the costs associated with avoiding norm violation.

In case the decision tree constructed expresses that a potential violation will occur (i.e. the tree predicts a violation) an intervention in the world can take place. The question of course is how to intervene. The basic idea is that only the input side of the agent can be influenced (for instance by sending a communication, or changing an observation). Hereby, an additional assumption is made, namely that the outcome of the reasoning process of the agent can still be influenced for a certain duration β by changing the input states. This allows the modification of the inputs of the agent during this interval β (given that transporting the new world information to the agent takes no time) and thus avoid the norm being violated. Deriving what input states to modify can be done by modifying the decision tree which has been constructed. This modification can be done by using the following algorithm:

Algorithm 2. Modifiable State Pruning

Start with X = source node

- 1. if X is not a leaf go to 2, otherwise if all nodes have been passed, go to 3.
- if node X is an element which is not modifiable, and this element is either true or false, then you remove the entire branch representing the truth value which is not observed. Follow the non-removed branch to the next node, set X to that node, and return to 1.

else if node X is modifiable, go to 1 for both the node when following the true and the node following the false branch.

 from all leafs that are left and labeled true (i.e. the decision tree indicates this branch resulting in violation of the norm) start with Y = parent node of this leaf and do the following: a. if Y only has one branch, remove the node and the branch that points towards this node, set Y to the parent node and go to a.
 else if Y has multiple branches, remove the branch that has just been taken.

If the result of this algorithm is an empty tree, it is unavoidable that the norm will be violated. Otherwise, the world can be modified such that the set of input states of the agent is identical to the set of states still present in the decision tree. The definition of whether an element is modifiable can be expressed as follows:

 $\text{modifiable}(\mathsf{E}) \rightarrow$

 $E \notin PrevState(a) \land E \in Ext(a) \land modification_time(E) < \beta$ Thus, an element is modifiable in case it is not part of a state in the past, and furthermore the modification time is shorter than the parameter β which has just been introduced. Figure 1 shows an example of a proof tree which has resulted from the ID3 algorithm. Hereby, the nodes represent the state name and the branches the truth value of this state.

Furthermore, it is given that both o_1 and o_3 in this tree are modifiable within duration β . In addition, it is given that prev(o_2) is false, o_1 is true, and o_3 is true. The resulting tree after application of algorithm 2 is shown in Figure 2.

The sets of states that can be reached and avoid violation according to this tree (i.e. all possible paths to the leafs of the tree) are referred to as AvoidViolation₁(a, n_a), ..., AvoidViolation_n(a, n_a). If n is greater than 1, one of the sets can be chosen based upon the costs of these modifications (whereby change_cost(s) indicates the cost to change input state s). Hereby, again an algorithm is specified for reducing the (already reduced) tree, in this case to one single option:

Algorithm 3. Costly State Pruning

For all nodes in the tree that still have multiple branches:

Select the node X with the highest change cost and remove the entire branch of the truth value which is currently observed to be the case on the input state of the agent.

In the case of the tree shown in Figure 2, the following desired situation would result from application of algorithm 3: {o1, prev(o2), \neg o3}, in other words, only o3 needs to be modified from true to false. Hereby it does not matter what the cost are since only o₁ can be modified.

An assumption of algorithm 2 is that there is merely one violation, which might not always be the case. Therefore, the possibility to address multiple norms is addressed as well. Hereby, it is assumed that for each norm that plays a role in society, a decision tree is present. The idea is now to combine these trees into one tree, whereby the leafs represent which norms will be violated. In order to build such a tree, take the set of all nodes from the decision trees (i.e. IndicationViolation(a) = IndicationViolation(a, n_1) \cup ... IndicationViolation(a, n_n)). Hereby the tree is constructed by iterating through all these elements as follows:

Algorithm 4. Creating Decision Tree for Multiple Norms

Start by constructing a source node of the tree which represents the ontological element in the first element of the set







Figure 2. Pruned decision tree

IndicationViolation(a). Construct two branches labeled true and false respectively. Set i to i=2 $\,$

- if i ≤ |IndicationViolation(a)| For each branch without a nodeattached: construct a node labeled with the state name without the truth value of the ith element in IndicationViolation(a). Construct two branches labeled true and false, and set i = i + 1 and return to 1.
 - else construct leaf nodes in the tree that represent the entire set of norms {NormViolationState(a, n₁),..., NormViolationState(a, n_n)} under investigation. Label these
 - by using the truth values of the different elements from the source of the tree to this leaf and the specific decision trees for the norms.

In order to now prune the tree, the costs of norm violation are taken into account. Assumed that for each norm certain violation costs for society are specified (violation_cost(n_a)). The idea is to minimize the costs for society first, and in case multiple options are still feasible, select the option which costs least to manipulate. Given these costs the following pruning algorithm can be applied:

Algorithm 5. Pruning Decision Tree for Multiple Norms (extension of algorithm 2).

- 1. see algorithm 2.
- 2. see algorithm 2.
- calculate for all leafs that are left in the tree, the costs of that leaf for the society (i.e. the sum of the costs of the norm violation sets that are labeled true in that leaf), and go to 4.
- 4. if there is more than one leaf left, select the leaf with the highest costs

if the highest costs are greater than 0, start with Y = parent node of this leaf and do the following:

- a. if Y only has one branch, remove the node and the branch that points towards this node, set Y to the parent node and go to a
- else if Y has multiple branches, remove the branch that has just been taken, and go to 4.

else go to 5.

else go to 5.

 if there is only one leaf left you are done else use algorithm 3 for pruning the remaining tree based upon the costs of changing an element.

CASE STUDY

In this Section, an evaluation is performed of the proposed approach within the domain of Criminology. Note that this evaluation has been conducted together with a criminologist. An important theory within Criminology, the routine activity theory (Cohen and Felson 1979), states that a crime will occur when a motivated offender meets a suitable target without a capable guardian being present. So to prevent crime from occurring one of the key aspects from the theory needs to be addressed. Punishing citizens that have violated norms can have a deterrent effect, and may alter the motivation of the offender. Another way to decrease the crime rates is to make sure that capable guardians are present. For example police surveillance, parking lot attendants or surveillance cameras and alarm systems. Further, one can try to make sure to not be a suitable target, so not to wear an obvious notebook case, or a wallet in your pocket. The problem is however that all offenders have different preferences. Some do not have high standards when it comes to their target and are not scared by the idea of being locked away in prison. What can be done about these hardcore offenders? The type of offender that is life persistent, and who seems to never be able to stay out of trouble? In this case the focus is on this type of offender.

The algorithms as introduced before have been implemented in Java. The outcomes of the algorithms for the specific scenario introduced below have been generated using the Java implementation. Note that this evaluation only addresses learning from history for the sake of brevity.

Formal	Description	Modi- fiable
prev(presence_bank)	Bruce previously observed a bank being present	-
prev(quiet)	Bruce previously observed the bank located in a quiet area	-
prev(escape_route_ outside)	Bruce previously observed a good escape route outside	-
less_than_6_people	Bruce observes less than 6 people inside the visible area of the bank	20
escape_route_inside	Bruce observes a good escape route inside the bank	5
surveillance_cameras	Bruce observes surveillance cameras in the bank	-
alarm_system	Bruce observes an activated	5

alarm system (a red light

a visible weapon in the

visible area of the bank

Bruce observes a person with

15

blinking)

guardian

Table 1. Relevant input states of bank robber

Scenario Description

Bruce is a bank robber. The police have a large file on him, because he has been caught several times in the past. They have information on 20 attempts to rob a bank. However, not all of these banks actually got robbed. Bruce is known for always observing the bank for a while before he starts the robbery, usually at least 30 seconds. The police would like to know which aspects are relevant in his decision to rob a place. After going through his file they discover eight important input and previous input states (as shown in Table 1).

Table 1 describes the relevant input states, and the costs as calculated by the police of modifying the state. Hereby the previous states (observed outside the bank) are not modifiable. Note that these costs are not based on reality, but used as an example. Furthermore, some input states are not modifiable, e.g. the presence of surveillance cameras is not modifiable since this can not within he accomplished 30 seconds. The less_than_6_people state can be modified by quickly moving people from/to the back office of the bank which is not visible for Bruce. Furthermore, the escape_route_inside is modifiable by visibly obstructing/opening the door. The alarm system is modified by visibly switching on the blinking light of the alarm, or by switching it off. Finally, the guardian can be modified by the security guard or the personnel behind the desk hiding or showing a gun. Besides these input states there are two norms specified for this organization, namely robbery which specifies that the action of performing a bank robbery is not allowed, and shooting which specifies that shooting inside a bank is not allowed. In this case study, robbing a bank costs society 10,000, and shooting inside a bank (during a robbery) costs society 100,000.

Learning Based on History

After applying the ID3 algorithm for the robbery norm to the police history (using the full history as training set) the tree shown in Figure 3 results. Hereby, the branches represent the input states of Bruce whereas the leafs represent whether Bruce will rob (and thus violate the robbery norm) or not. The same process has been undertaken for the shooting norm, resulting in Figure 4.

Utilizing the Built Decision Tree

Due to his history Bruce got a parole officer assigned to him to track him during the day. One day the officer sees Bruce enter a bank. It is still early so there are not a lot of people on the streets yet. The bank lies near a highway entrance. So, once Bruce is outside the bank he can get away easily. The parole officer observes that there are 2 persons inside the bank and there is no guard present. The bank is equipped with surveillance cameras and an alarm system. Based on the trees built in the previous section, the advisor agent can derive that Bruce will rob the bank and use a gun to get away. After applying the algorithms introduced in the previous sections (algorithms 3-5) two input states are identified



Figure 4. Decision tree for shooting norm

that need to be modified to avoid violation of the norms, namely making the state less_than_6_people false, and making the input state guard true. These changes are performed by the parole officer, and as a result, Bruce will not rob the bank, nor will he start shooting. According to the criminologist this result indeed complies with what was to be expected based upon the definition of the scenario.

DISCUSSION

In this paper it has been shown how potential norm violation can be detected. Norm violation can occur in a society in case the enforcers of these norms do not have full control over all actions of the agents in the society. Potential norm violation can be detected using a decision tree to forecast these violations. Two approaches to derive such a tree have been introduced: (1) learning from history using a data mining technique (in this case the ID3 algorithm), and (2) by building the decision tree based upon the internal model which is present of such an agent. The prediction information can be used in advisory agents, or even norm enforcing agents (e.g. police/parole officers). Under the

assumption that these agents can receive the inputs of the other agents that will potentially violate a norm somewhat before they actually start processing, methods have been introduced that derive how this norm violation can be avoided. Such avoidance is accomplished by making adjustments in the world, and thus changing the input states of the agent. Several algorithms for deciding what states to change by looking at the costs of making this change and the costs to society have been specified as well.

The whole approach has been specified on a generic level, thus allowing reusability of the approach. The initial application of the approach presented in this paper is the domain of Criminology, in which it was shown to give accurate advice according to domain experts. An evaluation in other domains, for instance the domain of software agents, is future work.

One major issue within the approach presented is the scalability of the approach. Of course, agents can potentially have a huge number of input states, and thus the decision tree might become large, making the approach less efficient. Typically however, only a limited number of input states are relevant for norm violation, thus limiting the size of the decision tree (by pruning the tree). Furthermore, the size of the tree can also be reduced by pruning parts of the tree that always result in norm violation or no violation of the norm.

Within the domain of normative organizations, a lot of work has been done. In Searle (1995) a distinction is made between constitutive norms and regulative norms. Hereby constitutive norms create new states of affairs and regulative norms govern activities, for example expressing obligations and permission for performing actions. The approach presented in this paper addresses both types of norms. In e.g. Rubino et al (2007), Artikis (2003), and Esteva et al (2001) approaches for representing norm-governed multi-agent systems are introduced. This paper takes such specified norms as input and enables avoidance of violation of these norms. More specific for norm violation, in Beolla and Van der Torre (2008) procedural norms are discussed that can for example be used to motivate agents that play a role in recognizing violations or applying sanctions. In Vazquez-Salceda (2004) a formalism is introduced to detect, sanction and repair violations of norms. The approach presented in our paper is however meant to avoid this violation not to punish violations that have already taken place. This phenomenon can also be seen in society whereby e.g. probation officers track potential recidivists and try to avoid criminal behavior from occurring (Pease, 2002). Of course, the sanctions and repairs can still be very useful in case norm violation is unavoidable.

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SYSTEM FOR COMPARISON OF TRAFFIC CONTROL AGENTS' PERFORMANCE

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KEYWORDS

Road traffic control, agent comparison, optimization.

ABSTRACT

We present a method and software for comparison of different road traffic control systems based on using of software agents. In last years, the agent-based traffic control is often discussed. Many agents were designed, but there is no way how to compare them in the same situation. Our system is designed to allow placement of different traffic control agents in simulated traffic network. Afterwards, a simulation is run and performance of control agents is measured. The traffic conditions are the same for all tested agents; it is possible to use several different scenarios. Agents can be subsequently compared, because they had operated in the same conditions.

INTRODUCTION

Due to growth of road transportation, optimization of traffic control is explored by many institutions. Often it is too expensive or even impossible to build new or wider roads, so optimization of traffic control is the one of the most important ways to improve traffic situation in the cities. One of approaches to traffic control is using of software agents. In last years, many different control systems based on agents was proposed (some of them are described below, in overview of existing agents). However it is difficult to compare them against each other. Usually, it is possible to find comparison of control system with static control of the crossroads or comparison of different varieties of the system. But there is no simple way how to compare two systems described in different articles. Tests described in articles were performed on different simulators, used scenarios and traffic networks are also different. That is why we have decided to create system able to perform comparison of different agent-based traffic control systems in the same traffic network and with the same scenarios.

Approaches to traffic control

With development of automated traffic control, analytical methods to create time plans for traffic lights were developed. One isolated crossroad may be optimized (Guberinić et al. 2008), but optimization problem of control of the whole traffic network is too complex to be solved by methods of analytical mathematics. Instead of mathematical analysis, approaches of artificial intelligence are used. Proposed techniques include artificial neural networks, expert systems and different kinds of logical reasoning or evolution algorithms. One of the most discussed ways is based on software agents.

AGENTS IN TRAFFIC CONTROLL

Software agents

Concept of software agents has first appeared in seventies. Since then, lot of definitions were created. One of the most general was proposed by Stuart Russell and Peter Norvig (Russel and Norvig, 2002): agent is

Anything that can be viewed as perceiving its environment through sensors and acting upon that environment trough actuators. (p. 32)

According to this, agent has to be able to observe its environment and it has to have ability to influence this. Another, more specific description of agents can be found in (Wooldridge and Jennings, 1995). It describes agent as encapsulated computer system deployed in environment, which is capable of flexible and autonomous activities, in order to achieve a specific goal. Basic conditions implied by this definition are autonomy – the ability of agent to work without being control by other systems, reactivity – the ability to react to impulses from outer environment, sociability – the ability to collaborate with other agents in the environment and initiative – the ability to perform actions in order to achieve long-term goal. When agent fulfils these conditions, it may be called intelligent.

According to these definitions, software agents are natural way to model traffic controllers. At least two of these conditions are fulfilled by traffic lights controllers in dynamic traffic control. They have sensors to measure traffic on the controlled crossroad and they are able to interact with traffic by controlling traffic lights. Usually, they also work autonomously, without any central control. In more complex traffic control systems, controllers on crossroads are also able to communicate with each other, in order to share information about traffic in the whole controlled network. The ability to achieve long-term goals is not so usual in traffic control, most currently used traffic controllers are only reactive (able to react to current situation, without long-term planning).

Position of an agent

Agents in proposed control systems can be placed on several positions in traffic network. Most common are agents positioned on crossroads. There are two main approaches – one crossroad can be controlled by one agent, or each traffic lane can be control by a different agent. In more complex traffic control systems, agents may also be used to control roads, using variable message signs (Katwijk and Koningsbrugenn, 2002).

In agent oriented systems, not only control agents are used. Agents may be also placed on roads, to measure traffic characteristics, which are required by agents on crossroad to achieve better result (Roozemond, 2001). Because agents on crossroads are searching only local optimum, it is also possible to group agents into hierarchical, usually tree-like structure (France and Ghorbani, 2003). Agents on the bottom of the structure are responsible for optimization of traffic on one crossroad and agents on higher position are trying to improve traffic control from global point of view. Example of such structure can be seen at Fig. 1 – four crossroads are controlled by agents, two of them are using road observation agents to gain information about situation in front of the crossroad and all of them are controlled by one managing agent in order to optimize global criteria.



Figure 1: Positions of Agents

Structure of agent

Abilities of agents and tasks they will be able to solve are highly dependent on structure of agent, but some parts are common for all types of agents. Agent has to be able to observe surrounding environment, thus it has to have module able to obtain data from real hardware sensor. It also has to interact with its environment trough actuators. And inside agent has to be a program, capable of selecting action for actuators according to state of sensors (general scheme is on Fig. 2).

We can divide agents to two main groups – deliberative agents and reflex agents. This dividing is based on

General scheme of agent



Figure 2: General Scheme of Agent

agent's ability to create inner model of surrounding environment.

Simple reflex agents are not equipped with internal model of environment. Instead of that, they are able only to observe current situation and react accordingly. This approach limits agent's ability to plan future activities. On the other hand, reflex agents are simpler, not so hardware-demanding. They are effective especially when they are operating in the groups (Brooks, 1991).

Deliberative agents are able to create internal model of the surrounding environment. Thus, they react not only to current state of the environment, but also to its past states. Due to this, they are able to make more complex plans, but they requires more complex internal structure, than reflex agents.

The most common model of a deliberative agent is called Belief-Desire-Intention (BDI). In this model, agent is composed from three main parts. Model of surrounding world (possibly including knowledge about other agents) and rules allowing predictions about changes of world after applying some actions are called belief. Using of term "belief" also shows, that agent's belief don't have to be true. Agent's goals, utility function or other mechanism used to choose the best action are called desire. And actions already chosen to be performed are called intentions. BDI model is wide spread and there is a lot of tools allowing implementation of own, BDI-based agents (such as Jadex).

It is important, that all type of agents are using sensors to gain information from the environment and has actuators to interact with the environment. Thus our comparison system has to have interfaces for both of them. On top of that, agents may need to interact with other agents or be grouped in a hierarchical structure, so communication interface also has to be part of comparison system.

Overview of existing agents

In this section, we want to briefly introduce four of newly proposed agent systems, to demonstrate their versatility.

Hirankitti and Krohkaew (2007) proposed reactive agent for control one crossroad. This agent is using information about traffic situation in front of crossroad and also information about free capacity of roads behind crossroad. It is using set of rules to choose order and duration of signals. This agent may be used also to control isolated crossroads.

Danko Roozemond (2001) designed system based on three types of agents. Each crossroad is controlled by agent and crossroad control agents are grouped and managed by managing agent. If it is necessary, roads are observed by road segment agents and passing information to crossroad control agents (see Fig. 1, where similar system is shown). Crossroad control agents are able to learn and to control crossroad they are using not only information about current state, but also their knowledge of its history. Managing agent is giving suggestion to crossroad control agents, in order to search for global optimum.

Mizuno, Fukui and Nishihara (2008) created system of collaborating agents, controlling crossroads. Their agents are sharing information about movement of vehicles, in order to dissolve congestion. Using information about distance between crossroads and about number of vehicles waiting at adjacent crossroads, agent predicts number of vehicles, which will arrive in near future. They are effective only if they are used in the whole traffic network, they cannot be used to control isolated crossroad.

France and Ghorbani (2003) proposed to use hierarchical structure, with crossroad control agents and managing agents, responsible for the whole areas. If there is a lot of managing agents in the network, they also may be grouped and controlled by managing agent of higher level. Crossroad control agents are creating control strategies for crossroads (with regards only to local criteria) and send them to managing agents. Managing agents are creating their own strategies, with regard to global criteria and confronting them with strategies from crossroad control agents. If there is a huge difference, they create new strategy to reduce this difference and send it to the crossroad control agent. Both crossroad control and managing agents are using rule-based expert system in order to optimize control strategy.

COMPARISION SYSTEM

Comparing different agents is a difficult problem. Usually, each agent is described with some tests of its performance. Due to this, there is no simple way how to compare two agents from different articles. To make convincing comparison, three main conditions need to be fulfilled.

- Compared agent systems have to operate in the same traffic network. Some agents are tested only in very simple conditions, such as two or more crossroads on one road. In real world we need to deploy them in more complex environment.
- Traffic situation used for comparison has to be the same for all compared agent systems. It is also necessary to compare both agent systems in wide spectrum of different traffic conditions. For example agent in (Hirankitti and Krohkaew, 2007)

is effective in non-crowded road, but in crowded road, its effectiveness is decreased. Traffic condition should change several times during test, to test agent's ability to adapt.

• The same simulation engine should be used, to prevent ambiguity from possible mistakes caused by simulator. For example in some types of carfollowing simulators car can freely pass through vehicles in transverse lanes in crossroad, while in simulators based on cellular automatons this behavior is not possible.



Figure 3: Schema of Comparison Module

We speak about comparison of traffic control agents, but the same system may be used to compare any kind of traffic control, which is able to use our interface. It is not important, if traffic control algorithms are fulfilling any of conditions given in introduction part they only have to be able to collaborate with described interface.

Simulator

We are using JUTS (Java Urban Traffic Simulator, Hartman, 2003) to test agents' performance. JUTS is using discrete, time-stepped simulation. Each step is equivalent of one second in real world. Model of roads is based on cellular automaton. Simulation is composed from roads, divided to lanes. Lanes are modelled as arrays of cells, which can be free or occupied, depending on presence of vehicle or obstacle Roads are connected by crossroads. Vehicles are moving trough network in steps.

Vehicles in JUTS are not equipped with the ability to find their path through traffic network. Instead of that, two methods of vehicle routing may be used. The first one is using prepared paths for vehicles, the second one is based on using pseudorandom numbers to determine turning of vehicles on crossroads. If the first method is used, vehicles are following prepared routes. Typical example may be travel of vehicle from residential area to centre of the city in the morning and return in the evening. Data for preparation of such routes may be obtained from sociological surveys; it is difficult to obtain them automatically. Method of pseudorandom numbers is based on statistics collected on each crossroad. For each lane leading to crossroad, vector of turning probabilities for other lanes is created. Each member of vector represents probability, that vehicle will turn to the corresponding lane. These data may be obtained from automatic sensors placed in lanes on each crossroad in the network.

In JUTS, prepared routes are used mainly for simulation of public transportation, but it is also possible to use them for any other vehicles, if necessary. Method based on pseudorandom numbers generators is used by most of vehicles

Agent support

To connect agents with simulation, two types of agent container are implemented in the JUTS. First and more important is a container for crossroad control agent. It provides access to all traffic lights in the crossroad and to information about lanes leading from and to crossroad. Agent may use this container to obtain information about traffic situation in upstream lane. Because some agents needs also information about downstream, container is able to explore possible paths in crossroad and find all downstream lanes belonging to one upstream lane/traffic line. Second type of container is designed only to control one traffic lane; the whole crossroad would be then controlled by several collaborating agents. Lane container allows access to traffic lights of appropriate lane and to information about upstream and all downstream lanes. In current implementation, we allow using only one type of container - agents may control whole crossroads or lanes, but combination is not possible.

Containers also provide methods to search other agents in the simulation. In JUTS all objects are marked by ID numbers. Because agents are controlling specific objects, they are using their ID's. Thus, agent may be found by ID of controlled crossroad or lane. If this ID is not known, container is able to find ID's of neighbour agents, if they exists.

Implementation of two more containers is now being prepared. These will be a road container and group container. In some multiagent control systems, road agents are proposed to observe situation on the road and inform crossroad controlling agents about it (this is used in (Katwijk and Koningsbrugenn, 2002) or (Mizu et al. 2008)). Originally, we intended to emulate this only by measurements in appropriate lanes, carried out from crossroads. But for two reasons, we decided to use agent container instead. At first, road agents may be also designed to work with variable speed limit signs, according to their own plans or to request from crossroad agent. And the second reason is possible using of distributed computation. Using of agent container will allows us to use existing methods for communication, if measured road and crossroad will be distributed to different nodes.

Group container will be used for managing agents, if they are necessary. In some multiagent traffic control systems (for example in (Roozemond, 2001) or (France and Ghorbani, 2003) hierarchy of managing agents is used. Container will allow creating and managing group of crossroad agents or other managing agents, if more complex structure is used. It will provide methods to send messages to subordinate agents or to broadcast to whole group. This broadcasting has to be invoked by an agent in the group container – if one of subordinate agents needs to broadcast to the whole group, it is allowed only to send message to managing agent and it can decide if this message will be broadcasted or not.

Communication

Both containers provide also support for communication among agents. The crossroad container is able to send message to any specific crossroad, to multicast message to all neighbour crossroads or to broadcast message to all crossroads in simulation. The lane container can send message to another specific lane container, multicast to all lane containers in one crossroad or broadcast to all lane containers in simulation. Because distributed version of JUTS is developed, it is important to communicate only trough prepared methods, otherwise agent will not be able work correctly in distributed simulation. Messages are marked by its senders and they may have assigned priority. They are stored in priority queues in the container until they are read by agent (they cannot be lost or overwrite by newer message).

Measurements

All the measurements are provided by a statistics collector. Collector has full access to all objects in simulation map and it is able to obtain all kinds of information available in simulation. Lanes and crossroads in JUTS are creating their own statistics, such as long-term average vehicle speed or flow and they can be made accessible to agent containers trough statistics collector. The statistic collector is also able to detect queues and measure its lengths or collect statistics as an actual average speed of traffic density. Samples may be taken regularly, according to prepared plan – this is useful to evaluate agents' performance at the end of simulation. Collector is also able to take sample on request from agent container.

Statistics collector can also access to information from vehicles, not only from traffic network. It can measure average time they spent in simulation, by waiting in queues or how long they are waiting in the last queue. These data cannot be easily obtained in real world, but they are used in some proposed control agents (Balan and Luke, 2006), (Hoar et al. 2002).

Simulation control

Simulation control is used to automatically run prepared scenarios with different agents. Because amenities of dynamic traffic control are apparent mainly when traffic flow is not static, it is necessary to change settings of vehicle generators or probability of switching on crossroads. These changes are described in scenarios. Each scenario contains its length (in time steps, which corresponds to seconds), changes of pseudorandom number generators settings (which are used in vehicle generators and at crossroads) and time when change should apply. Settings of crossroad switching probabilities may be used even to simulate an accident, to test if agent is able to deal with sudden vast changes. Vehicles in JUTS are not able to search way in traffic network, so operator has to prepare the whole accident scenario, including paths used by vehicles to avoid accident. Simulation control ensures that changes will be applied after given amount of time. It is also possible to set seed of pseudorandom generators, thus achieve an identical scenario.

This module can be configured to execute several runs with different scenarios and agents and to summarize results of each run to xml files.

Comparison of agents

To compare agents' performance, results' comparator is using data obtained from the statistics collector. Compared values and places of their measurement have to be set before the simulation is started. There are three types of criteria used to evaluate traffic control of crossroad in (Guberinić et al. 2008) - criteria based on capacity, criteria based on queues and environmental criteria. Because our simulator is not designed to observe fuel consumption or CO, CO₂ and other pollutants dispersion, we focus only on first two. Capacity criteria are observing amount of vehicles passing through crossroad. There is a detail description in (Guberinić et al. 2008) how to compute maximal capacity of crossroad, which can be compared to achieved amount of vehicles. Queuing criteria are observing delay of vehicles in crossroad, caused by red signal or by insufficient capacity of crossroad.

Criteria for global evaluation may be based on average values obtained from each crossroad, but it is possible to use other information. The aggregate waiting time of vehicle on all crossroads can be measured. If vehicles are using static paths, it is possible to embrace average time spent by travelling, if random numbers generators are used, the same role is fulfilled by average time spent by vehicle in simulation. It is also possible to focus on situation on roads, not only crossroads. Average speed or traffic density may be used.

It is important to know, that not only selection of criterion, but also selection of places where it will be measured is important. For example on junction of two main roads, the agent may try to treat them both as equal or to prefer one of them – which of course leads to deterioration of measured criteria in the other road.

EXPERIMENTS

In this part we show method of experiment used to compare performance of two traffic control systems. Each simulation experiment consists of four main parts – model of tested network, scenario, set of agents and their settings, and chosen criteria used to compare their performance. Selection of criteria is very important, because there is no general way how to tell if traffic control is optimal or not. For example agents (or traffic control systems) minimizing length of queues may not be optimal if average speed is observed. It is possible to observe more than one criterion, but then operator has to decide which of them is more important.

The traffic network model contains a full description of roads and crossroads. It cannot be changed during experiment. Even accidents and blocking of traffic lanes has to be done in scenarios. This is because vehicles in JUTS are not able to find their own way trough simulation map, so if the map is changed, prepared paths or turning probabilities has also to be changed. Because in our simulation only vehicles play active role, the model may be complex, number of roads and crossroads has only little influence on speed of computation.

Scenario contains description of vehicles in the simulation. Two most important parts are description of vehicle generators at the edge of simulated network and random numbers generators on crossroads, responsible for turning of vehicles. Contrary to traffic network, these values are changed during experiment, in order to determine ability of agent to adapt to new conditions. Data for scenario can be based on values measured in real world, or they may be prepared by operator. In this case, it is important to try scenario before experiment is performed, to check if it is suitable and it represents required situation (for example, wrong setting of vehicle generators may lead to rapid congestion of traffic network, wrong setting of crossroads may caused accumulation of vehicles in some parts of network). To test all abilities of control agent, several experiments has to be performed, with different scenarios. Agent capable for example of optimal control of uncrowded road may have problems with solving heavy congestions. Because plays an active role in the simulation in JUTS, scenario has the biggest influence on the speed of computation. With higher number of vehicles, simulation is getting slower.

Description of agents contains not only algorithm of each agent, but also their position and settings. Even if only one type of agent is used, agents from different crossroads must not be confused. Each agent has its own unique settings, which has to be prepared for crossroad controlled by it. Some types of agents are able to change these settings due to their learning mechanism, but in many cases at least some of setting is static and cannot be changed by agent itself. It may be only set of parameters, as preference of one direction or minimal and maximal duration of green signals, but some agents also requires preparation of signal phases or initial estimates of traffic density in all controlled lanes. If agents are able to learn, they should be run in typical scenario for the area, in order to give them initial state.

Unfortunately, it is often, that method how to set similar properties is not described in articles with descriptions of agents. Even a very efficient agent may give a poor performance, if these settings are incorrect. Settings also cannot be part of scenario, because agents are supposed to act autonomously, without an outer control. Another important thing is hierarchy of agents. If hierarchical structure is used (for example (Roozemond, 2001) or (France and Ghorbani, 2003)), it also has to be part of description of the experiment. Even with the same setting of each crossroad-controlling agent, results may be different if they are grouped differently. It is caused by managing agents. They are helping to find global optimum within the group, so in different groups agents will be working on search of global optimum for different parts of the network.

The last part of description of experiment is selection of criterions and position of their measurement, if necessary. It is possible to observe and compare any amount of places in the network, as well as global statistics. Selected criteria are not effecting the work of agents, they are used only for their comparison.

Evaluation of experiment is basically evaluation of hypothesis that according to chosen criterion in given network and scenario, optimal control is achieved by one of used traffic control agents. Because this hypothesis is valid only for the whole experiment, it is important to perform several experiments to determine quality of control of one agent.

Proposed scenarios

In this part, several basic scenarios and the way how to create them is given. These scenarios may be used to compare performance of all described traffic agents.

The most basic scenario is steady traffic flow with static density. It shows ability of agent to ensure traffic fluency or priority of important roads. No changes are done during experiment, but several experiments with different densities should be performed to see capacity limits of agents and traffic network. In this case, even with very simple agents, traffic congestions are caused more by maximal capacity of the network, than by insufficient ability of agent to control network.

Similar experiment is dealing with fluctuating traffic flow. During experiment, density of traffic flow raises and drops several times. A typical example from the real world is a control of roads leading from residential areas to the city and back – during morning, there is a lot of traffic to the city and only few cars are going in opposite direction. During evening, situation is inverted; heavy traffic is in the direction from the city. This scenario shows ability of agent to adapt to different situations and to control traffic for the whole day. The period with unchanged traffic flow should be long enough in order to simulate real situation.

Ability of agent to solve congestions may be tested by heavy traffic flow, causing congestion at the beginning of the experiment. It may be created only on main road or on crossing of two main roads and propagates itself to the whole network. Some agents, as (Logi and Ritchie, 2002) are created specifically to solve congestions.

The last important scenario is reaction of agent to accident or any other type of roadblock. In this scenario, vehicles generators are working in the same manner as in normal situation, but turning probabilities or paths has to be changed. During preparation, it is necessary to decide where detour will be and change turning probabilities in all affected crossroads, not only on the one with accident. This shows ability of agent to react on rapid change of situation in controlled crossroad.

Example of experiment

As an example, we have tested agent proposed by Hirankitti and Krohkaew, and compared it to vehicle actuated signal control (simple dynamic system, capable only to prolong duration of green signal if vehicle is detected in the lane). Part of testing map is shown at Fig. 4. Results were measured at highlighted crossroad at bottom right, as a criterion we choose average length of queues in each lane at the end of red signal. Lanes are denoted by letters a. f.



Figure 4: Screenshot from simulator and scheme of tested traffic network

We have tested two scenarios with the same number of simulation steps. In both traffic density was changed several times. In first scenario, three peak of denser traffic were created, in second six peaks. During peak traffic density was two times higher between peaks.

Both control systems were set to prioritize main road (lanes a,b,d,e). It means longer green times were allowed in these lanes.

Results from both scenarios can be seen at Fig. 5. We may see, that Hirankitti's and Krohkaew's agent achieved better results (shorter queues, with the same traffic density means, that more cars were able to pass crossroad during each signal cycle), especially in the first scenario. With higher traffic density in second scenario, result of both systems is similar. This is caused by approaching to maximal road capacity.

Better results of VHJK agent are caused by better utilization of space in roads. VASC is only able to change duration of phases, according to number of vehicles in lanes with green signal. If there are vehicles only in one lane, VASC is still keeping the sama signal

phase. VHJK is able to deal with such situation. If vehicles are only in one lane (for example a at Fig. 4), VHJK is able to find directions, which can have green signal in the same time (direction f at Fig. 4) and activate them in the same signal phase. Thus, if such situation often occurs, more vehicles can pass crossroad in constant time.


Figure 5: Comparison of VASC and VHJK for first (top) and second (bottom) scenario

FUTURE WORK

Our priority is to implement a number of proposed control agents and perform comparisons to determine their abilities and weak points. Before comparison, we need to validate our implementation of the agent's systems, by performing tests from the articles, where the agents are described in. If the results we obtain from our simulation are similar as the results from the articles, we assume that our implementation is valid.

One of problems in the traffic control is a decision what should be optimized. There is lot of criteria, and no clear way how to tell which is more important than the others. Designers of traffic networks and control systems may try to minimize length of queues or amount of time spend in congestions, or to maximize amount of vehicles passing through network during one hour, fluency of car movement or average speed of vehicle (other used criteria may be seen in (Guberinić et al. 2008)). Our goal is to find suitable method, which allows automatically decide which way of traffic control is at least semi-optimal for specified purposes.

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O D i M: A MODEL-DRIVEN APPROACH TO AGENT-BASED SIMULATION

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KEYWORDS

Agent-Based Simulation, Model-Driven Development, Meta-Modelling, Domain Specific Visual Languages.

ABSTRACT

Model-Driven Software Development (MDD) is a software engineering paradigm that uses models as a means to specify, test, verify and generate code for the final application. Domain-Specific Visual Languages (DSVLs) are frequently used as high-level notations to specify such models, and hence the systems to be built. In this way, developers work with concepts close to the domain, and need not be experts in lower-level notations, thus increasing productivity.

In this paper we show the application of MDD to agentbased simulation. In particular we present the design of ODiM, a DSVL for Modelling and Simulation of Multi-Agent Systems. The language is made of four different diagram types, used to define agents' types, their behaviour, their sensors and actuators and the initial configuration. We have built a customized modelling environment integrated in Eclipse, and a code generator for MASON, a Java-based agent simulation language which allows the visual simulation of ODiM models.

INTRODUCTION

Model-Driven Development (MDD) is a software engineering paradigm which seeks increasing quality and productivity by considering models the core asset in software projects (Stahl and Volter 2006). They are used to specify, simulate, test, verify and generate code for the final application. Domain Specific Visual Languages (DSVLs) are graphical notations constrained to a particular domain and play a cornerstone role in MDD (Kelly and Tolvanen 2008). DSVLs provide high-level, powerful, domain-specific primitives, having the potential to increase productivity for the specific modelling task. Being so restrictive they are less error-prone than other general-purpose languages, and easier to learn, because the semantic gap between the user's mental model and the real one is smaller.

In computer modelling and simulation, systems are described using appropriate languages and notations for the purpose of virtual experimentation (Zeigler et al.

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) 2000). Some of the disciplines that traditionally have used simulation as a research or decision-making tool include physics, mathematics, biology and economics. Lately, simulation has become popular in the social sciences with the emergence of agent-based simulation techniques (Gilbert, Troitzsch 1999). In this paradigm, the main concept is the agent (Jennings et al. 1998) (Wooldridge 1999), which can be defined as a "computer system, situated in an environment, which is able to perform flexible and autonomous actions to achieve its design objectives".

In agent-based modelling and simulation "*macroscopic*" phenomena emerge by the actions and interaction of elements at the "*microscopic*" level (Alfonseca and de Lara 2002) (Bonabeau et al 1999). Thus, the classical macro-level approach of representing systems as differential equations is no longer used. Instead, the variation of the quantities in the model is obtained from the explicit modelling of the individual elements. This presents several benefits, such as a deeper insight and understanding on the phenomena to be modelled.

Even though agent-based simulation is useful for a variety of disciplines, models are frequently described using low-level languages, often extensions of general purpose object-oriented programming languages like Java (Minar et al. 1996) (Luke et al. 2005). In this respect, our goal is to use MDD techniques to provide intuitive, visual notations for describing agent-based models in a precise way in order to facilitate the construction and execution of simulation models by non-programmers. For this purpose, we have designed a DSVL for modelling multi-agent systems called ODiM. The language is made of four different diagram types, used to define agents' types, their behaviour (based on state-machines), their sensors and actuators and the initial configuration. Thus, ODiM is tailored to agents of reactive type (Brooks 1991). We have built a customized graphical modelling environment integrated in Eclipse (Eclipse GMF 2009), and a code generator for MASON (Luke et al. 2005), a Java-based agent simulation language which allows the visual simulation of ODiM models. In this way, users of ODiM, just deal with a graphical notation, and do not need to be proficient in any low-level programming language.

DOMAIN SPECIFIC VISUAL LANGUAGES

DSVLs are constrained notations tailored to specific domains and needs. MDD uses DSVLs in wellunderstood domains, where high-level, intuitive primitives can be identified to describe the problem at hand. Thus, the users of the DSVL are more productive as they are familiar with the primitives of the DSVL, the mental gap from the model to the problem is smaller, and no low-level, general purpose-languages are needed for encoding the solutions. In these restricted domains, code generators can be built to generate most of the code of the final system.

One way of specifying a DSVL is through a metamodel, which is model of the DSVL (abstract) syntax, and describes its main concepts. Meta-models are often specified using visual languages, such as UML class diagrams, and are usually complemented by textual constraint notations (like OCL) expressing additional language constraints. As an example, Figure 2 shows a part of the meta-model for the state machines that express the behaviour of ODiM agents. The meta-model describes that agents have behaviour, expressed through state machines. These contain a list of states, which can be normal, initial or final. States have transitions, which have a guard and an action. By means of OCL restrictions, we have specified that there is a unique initial state, which cannot receive incoming transitions, and that final states do not have outgoing transitions.



Figure 2: State Machine Meta-Model (partially shown).

The definition of a DSVL requires also a concrete syntax, specifying how each element is visually represented. In the simpler case, this is done by assigning graphical icons to classes in the meta-model and decorated arrows to associations. In the example of Figure 2, states are represented as ovals with the name inside, and transitions as edges. Figure 9 shows an example of a state machine. Meta-modelling tools like AToM³ (de Lara and Vangheluwe, 2002), or GMF (Eclipse GMF 2009) are able to generate customized modelling environments for a DSVL given a meta-model and a description of its concrete syntax.

In addition to the syntax, it is necessary to specify the DSVL semantics, its meaning. One way to do this is to use a denotational style, relying in some other language for which the semantics are already defined. This is the approach we follow, by generating code for the MASON simulator (Luke et al. 2005).

Finally, DSVLs may also be used to describe complex systems that include different aspects or concerns. The complexity of these systems makes a common practice its specification by means of a set of smaller diagrams (called *views*) instead of including all the information in a single, monolithic one. Each one of these smaller diagrams is more comprehensible and cohesive, describing some feature of the system from a specific viewpoint. Thus, some DSVLs offer different diagram types in order to describe the various aspects of the system. These notations are known as Multi-View Visual Languages (MVVLs) (Guerra et al., 2005). For example, the UML notation proposes a set of diagram types to describe the static and dynamic aspects of the application. Note how, MVVLs are not described in a separate way, but the language is described through a common meta-model, which includes the meta-models of the different diagram types and their relation. In our case, the ODiM language is made of four different viewpoints to describe the agent structure, sensors and actuators, the agent behaviour and the initial configuration. The language is described in next section.

THE O D i M LANGUAGE

ODiM is a DSVL oriented to modelling and simulation with multi-agents. In a declarative way and through high-level visual notations, ODiM allows modellers to build simulation models based on the multi-agent approach. Thus conceptually, the main element of the language is the (embodied) *agent*, with the salient feature that every interaction has to occur through sensors and actuators.

We present the language through a simple simulation model, taken from (Miñano and Beltran, 2004). The model consists of a two-dimensional micro-world populated by agents, obstacles and goals. The microworld is a multi-agent system where agents interact with their environment and other agents in order to reach long-term goals. Goals are static entities, sought by agents. They are called "long-term goals" because they are usually at a distance from agents, so it takes a certain amount of time for the agents to reach them. Goals have yellow colour, each one occupies one patch in the environment, and initially, they are scattered randomly. Obstacles are areas composed of contiguous patches that cannot be occupied by agents and which agents cannot see through. They have black colour, and are also randomly distributed. As in ODiM interactions are embodied, goals and obstacles have an actuator to exhibit their positions in the micro-world as twodimensional coordinates and the colour of their surface. This actuator generates a visual stimulus which can be perceived by the sensors of the agents.

Agents can move around and look for goals. Every agent can sense and act independently, based on a set of rules that neither explicitly indicate how to reach the goal nor provide a predefined sequence of steps to be followed to reach it; instead, it only tells the agent how to respond to obstacles and other entities in the environment. These rules are described in the state machine of each agent.

Agents have two-dimensional coordinates that specify their positions, and headings that indicate the direction of their movement. An agent can move one cell or patch per time unit in any direction relative to its current position (north, northeast, east, southeast, south, southwest, west, or northwest). An agent heading is defined as the angle between the linear path that links its positions at times t-1 and t and the horizontal axis of the micro-world. Agent coordinates are initially set at random. Agents are also endowed with perception, which allows them to scan their neighbourhood in order to identify different kinds of entities (goals, obstacles, and other agents) and this is represented by a sensor. This sensor acts as the vision sense of agents and is designed to react to the visual stimulus generated by actuators of goals and obstacles. An agent state is defined by two values: (i) Explorer, meaning that the agent is looking for goals and then it is shown in green colour and (ii) Rich, when an agent reaches a goal, and it is shown in blue colour. Rich agents do not react to other entities, but stay in the position where they found a goal. When an agent detects a goal, it remembers its position and goes straightforward to it. If an obstacle is detected, the agent turns around 90° to avoid it. Finally, an agent changes its colour depending on what entity is detected: magenta when a goal has been detected, orange for a rich agent, brown for explorer agents and cyan when an obstacle has been detected.

Next subsections present the different ODiM diagrams, using the previous model as illustration.

The Agent's View

The agent view allows describing the internal structure of the agents. An ODiM agent is made of a name, basic properties and properties representing perception and action devices called *widget properties*. Basic properties are of some predefined primitive type such as *Boolean*, *String*, *Integer* and *Double*. Widget properties are sensors and actuators. These are devices allowing interaction between agents and their environment. This view also allows referring to the agent state machine, used to specify its behaviour. Figure 3 shows the metamodel of the agents' view. In ODiM the simulation environment is modelled as an agent, hence every model has initially an agent called *Environment*. As with all agents, we may associate a state machine to the environment agent and define a specific behaviour for it.



Figure 3: The Agents Viewpoint Meta-Model.



Figure 4: The Micro-world Agents in O D i M.

Figure 4 illustrates the agent structure of the example. The agent Agent has properties x and y that define its position. Property *color* is encoded as an integer with the RGB value. Property *reachAGoal* is used to manage the status of the agent. Initially, its value is false, but when an agent reaches a goal its value is set to true. Property *headingAngle* indicates the direction of movements and its initial value is 90° (i.e., north).

Sensors and Actuators: The Widget View

Inspired by the biological models of perception and communication, the interaction between agents and its environment is defined through the generation of stimuli and the response of the agents and the environment to those stimuli. An agent interacts with its environment and other agents through actuators and sensors that we call *widgets*. The *widgets view* describes the structure of actuators and sensors, the stimulus that can be generated by an actuator and the events produced by sensors as a reaction to the stimulus perception in the environment. Figure 5 shows its meta-model.



Figure 5: The Widget Viewpoint Meta-Model.

Actuators. An actuator is a kind of device that exhibits properties by generating stimulus. These properties may be characteristic of the actuator or internal agent properties. The *Stimulation Rate* in class *Actuator* is the frequency with which a stimulus is generated and propagated into the environment by an actuator. The frequency can be *on demand*, *permanent* or *on time intervals*. In the first case, the generation of stimulus takes place by an explicit invocation of a primitive action in the actuator. The execution of this action creates an instance of the stimulus, which will be added to the stimulus queue of the simulation environment. Once into the environment, the stimulus is available to be perceived by the rest of the agents or the environment itself. The second case (permanent stimulation) refers to the constant generation of stimulus by the actuator, at each simulation time. Finally, in the third case (on time intervals), the stimulus are generated by the actuator every certain number of time steps.

Each time an actuator generates a stimulus, the values of the properties that the actuator exposes are copied to it. Figure 6 illustrates the concrete syntax of an actuator in ODiM. The actuator *SkinActuator* is designed to expose the position of the agent in two dimensions (x,y coordinates), as well as its colour, encoded as an integer value. The information is exposed through a *VisualStimulus*. The frequency generation of the stimulus by the actuator is on time intervals because *stimulusRate* = 3.



Figure 6: SkinActuator for Micro-world Example

Stimulus. A stimulus is a sensorial phenomenon immersed in the simulation environment and external to the agents. It represents a perceptible change in the environment. A stimulus may influence the behaviour of the agents and their environment, depending on the perception sensitivity of its sensors to that stimulus, and the interpretation and response of the agents. A stimulus in ODiM has a an intensity, which is the time during which it is available in the environment so that it can be perceived by all agents with sensors equipped with sensitivity to the stimulus. A stimulus can have permanent or limited intensity. In the first case, the stimulus is stored in the stimulus queue of the environment and is available at all times in the simulation. In the second case, the stimulus is available in the environment during the time of the simulation specified by the value of the intensity property.

Figure 7 illustrates the concrete syntax of a stimulus. The stimulus *VisualStimulus* is generated on time intervals by the actuator *SkinActuator* and it can be perceived for all agents equipped with sensors of type *VisionSensor*, with a perception frequency of 2 simulation time units. Once the stimulus *VisualStimulus* has been generated, it will be available in the simulation environment during the next 3 simulation time units.



Figure 7: VisualStimulus in the Micro-world Example.

Sensors. A sensor is a device that provides agents with perception capabilities, allowing them to perceive stimulus immersed in the environment, generated by actuators of other agents. A sensor is composed of properties that define its internal structure. A sensor perceives stimulus according to a sampling rate called *Perception Rate.* A sensor can be designed so that it is sensible to stimuli under certain circumstances, which is expressed through a Perception Guard. This is a boolean expression representing a condition that must be met for that sensor to perceive the stimuli to which its capacity of perception was designed. The expression may contain references to the properties of the sensor, to the properties of the type of stimulus that the sensor can perceive, language primitive functions and constant values for primitive types in the language. Each time a sensor perceives a stimulus, it notifies the agent through the generation of events. These act as a mechanism for communicating information from the outside to the agent controller, represented by the state machine.



Figure 8: VisionSensor in the Micro-world Example.

Similar to actuators, sensors can have an on demand perception, permanent or based on a time interval.

Figure 8 shows the definition of the sensor *VisionSensor* designed for visual perception, that is, to detect stimuli of type *VisualStimulus*. Properties *x*, *y* and headingAngle in the sensor are fed with the position and heading angle by the owner agent. When the guard expression is evaluated to true for some stimulus instance in the environment, then the sensor generates an event of type *SEE_OBJECT*. The event is sent to the internal event queue of the agent owner of the sensor and is available for the transitions in the state machine. Notice that the expression in the perception guard has nothing to do with any complex programming language. It just has mathematical terms and references to the properties of the sensor and the stimulus it perceives.

The Behaviour's View

The behaviour of agents is based on a reactive architecture (Brooks, 1991). The agents react to stimuli received through its sensors and interact with other agents and its environment through its actuators. The only information available to agents is an internal queue of events, produced by sensors. These events are no more than a copy of the information available in the environment, which is propagated through the stimuli generated by other agents or by the environment. The behaviour of an agent is defined visually using a state machine. This represents a single and independent thread of control, which determines the agent internal state in an instant of the simulation. Figure 9 shows the state machine for the agents of the example.



Figure 9: State Machine for the Micro-world Agents.

The agent state machine has a high dependency on sensors and actuators. It can modify the agent's internal state, made of the values of each one of its properties, the state of its sensors and actuators, and the state of the queue of events generated by each one of its sensors. The state of the sensors and actuators is determined by the values of each one of its properties. The properties of an agent and its sensors and actuators are visible to the states machine of the agent. An agent can modify the properties of its sensors and actuators, but those will not be able to change the properties of the agent.

The transitions occur instantaneously and modify the current state of the machine moving it between states. A transition is enabled if the following conditions hold: (i) the source state of the transition is the current state on the state machine, (ii) the trigger event of the transition has been generated by any sensor and is available in the internal event queue of the agent, and (iii) the guard of the transition is evaluated to true. Once a transition is enabled, it is fired, leading to the execution of the associated actions and a change of state. If several transitions are active, we use the priority of the sensors that have generated by the sensor with higher priority. If there are multiple sensors with the same priority, a transition is chosen randomly.

In ODiM, transitions may include time events (with syntax time(t)). Similar to DEVS (Zeigler et al. 2000), time events determine how much time the agent must wait in a state in the absence of external events. The time can be a constant or be defined by a property.

The Instances View

This view allows the configuration of the initial state of the system (e.g. positions of agents, obstacles and goals, etc). By space limitations, we omit its description.

THE MODELLING ENVIRONMENT

We have built a modelling environment for ODiM, and integrated it in the Eclipse framework. For this purpose, we have used the GMF (Eclipse GMF 2009) toolkit, and designed a MVVL with four different views. Figure 10 shows a screenshot of the environment.



Figure 10: Modelling Environment for O D i M.

Code Generation for MASON

MASON (Luke et al. 2005) is a single-process, discrete event simulation core and visualization library written in Java, designed to be flexible to be used for a wide range of simple simulations, but with a special emphasis on swarm multi-agent simulations. In MASON, agents are "brains" which may or may not be embodied. In the latter case, we call them embodied agents. Note that, as the simulation designer uses ODiM (where interactions are embodied), we force MASON agents to be embodied. MASON does not schedule events to send to agents; instead, it schedules the agent to be stepped (pulsed or called) at some time in the future. Hence, MASON agents implement the *Steppable* interface.

MASON can schedule Steppable objects to occur at any real-valued time in the future. However, we schedule the agents in ODiM in a discrete way. The Schedule may be divided into multiple orderings that further subdivide a given time step: agents scheduled at a given time but in an earlier ordering will be stepped prior to agents scheduled at the same time but in a later ordering.

MASON is written in three layers: the utility layer, the model layer, and the visualization layer. The former consists of classes that may be used for any purpose, e.g. random-number generators, data structures and other facilities. The model layer is a small collection of classes consisting of a discrete event schedule, schedule utilities, and a variety of fields that hold objects and associate them with locations. This code alone is sufficient to write basic simulations running on the command line. The visualization layer permits GUIbased visualization and manipulation of the model. For most elements in the model layer, down to individual fine-grained objects in the model, there is an equivalent "proxy" element in the visualization layer responsible for manipulating the model object, portraying it onscreen, and inspecting its contents.

Code generation techniques save time in projects, reducing the amount of tedious redundant programming. Code generators are powerful tools, but they may become very complex and hard to understand. One way to reduce complexity and increase readability of model compilers is to use templates for code generation. Java Emitter Templates (JET) (Eclipse EMF, 2009) is a tool provided by The Eclipse Modelling Framework (EMF) project that allows using JSP-like syntax to write templates expressing the code that needs to be generated. A JET template is a text file, from which JET generates a set of classes that contains the code needed for the generation. The JETEmitter class provides a convenient high-level API to transform templates and generate code programmatically. The generate method of the JETEmitter class combines template translation and text generation into a single step.

The strategy we have followed for generating MASON code is to build a set of JET templates that collect rules for translation between the ODiM simulation model and the programming model of MASON, combined with a framework (utility classes) built on MASON that supports its programming model. The supporting framework consists of a set of utility classes (AbstractAgent, AbstractSensor, AbstractActuator, AbstractStimulus, etc) that abstract the common operations for the main concepts in ODiM. As MASON agents are modelled by a Java class, implementing the interface Steppable, those classes are implementations of the class Steppable. The advantage of our strategy is that JET templates are simpler and easier to maintain than a specific, hard-coded model compiler.

Thus, agents, sensors, actuators, stimulus and the simulation environment are translated to MASON as classes which inherit from its corresponding abstract class in the supporting framework. For example, the agent *Agent* in the micro-world generates the class *MASONAgent* which extends from *AbstractAgent*. Basic properties are synthesized as private attributes whose data type has the proper correspondence with Java types. Widget properties are generated in the same way, but the attribute type is the corresponding class generated for the sensor o actuator. Stimulus and Events are Plain Old Java Objects (POJOS). In all cases, getter and setter methods are provided to have access to attributes.

The actions of the state machine of the agents are coded in the *step* method, which is executed at each step of the simulation according to the schedule of the agent. Instructions available for transitions in the state machine are supported by a set of language primitives as *scan*, *createAgent*, *generateStimulus*. Also, mathematical operations may be used.

Figure 11 illustrates an execution of the example, where we can see the adaptive behaviour of the agents to different entities inside the environment, according to the ODiM model.

RELATED WORK

Several agent-based languages can be found in the literature, like Swarm (Minar et al. 1996), Ascape (Inchiosa and Parker, 2002) and MASON (Luke et al. 2005). Most of them are libraries for object-oriented, textual programming languages. This requires the users to be proficient in programming tasks, and in addition, none of them is based on a graphical notation.

There have been some attempts to design graphical modelling notations for designing multi-agent systems. For example, the FIPA modelling committee is working on AUML, (Odell 2004). Although their aim is to be domain independent, in the area of simulation many domain-specific concepts are necessary (like sensors, actuators, stimuli, etc.). Thus, we believe creating a DSVL makes sense. Such DSVL has the goal of offering high-level, customized constructs for the task to be performed, as well as constraining the user as much as possible. Therefore, we believe that using a customized modelling notation for agent simulation, the user is more productive than using a more general one. Moreover, AUML is only a design notation, and thus the resulting specifications are not executable.



Figure 11: A step in the Simulation of the Example.

In (Muzy et al 2007), we developed a graphical notation for agents, where no code generator was provided, but only a mapping into DEVS (Zeigler et. al 2000).

CONCLUSIONS AND FUTURE WORK

In this paper, we have presented ODiM, a DSVL for agent-based modelling and simulation. The aim of the language is to provide high-level, visual constructs for building easily agent-based models that can be simulated by using MASON as a back-end. ODiM provides different diagrams to specify the different aspects of the simulation, thus making the design modular. We have built a customized modelling environment and a code generator for MASON, so that the user does not have to know any programming language. There are many possible lines of research. We are currently working in providing three dimensional graphical output forms, in extending ODiM so as to allow the control of agents with neural networks, and in developing further code generators, for example to synthesize controllers for real robots (Lego, 2009). We are also working on including library concepts and reusing facilities, so as to allow reusing already defined sensors, actuators and controllers.

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BIOGRAPHIES



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ON AGENT MODELLING AND SYSTEM SIMULATION OF SELF-ORGANISATION

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KEYWORDS

design, implementation and validation methodologies; multilevel simulation; self-organisation; multi-agent systems; system design; formal specification; empirical analysis.

ABSTRACT

Complex, natural, social, technological and economic systems have recently given rise to the need of a new paradigm for computational systems that are adaptive, can self-organise and exhibit emergent behaviour. The design of such systems concerns a homogeneous set of agents in which each agent receives an input and has to map it to a 'good' output, and where self-organisation emerges from the interaction between agents. Although general and simple, this concept is representative for a very wide spectrum of applications such as protocol design for large computer networks, design of collective robotics, and automative traffic engineering. Surprisingly, only a handful of recent research is aimed at a domain-independent (or: general) design of such systems. We propose as the solution for the design-problem a framework that tackles the local (agent) level formally and the global (system) level empirically. This allows us to do rigorous formal verification of the behaviour of the individual agents, as well as large-scale empirical validation of the system as a whole. Besides, it exploits the specific advantages of the approaches regarding the scale of the system: formalisation is good for small systems, while simulation works well for (very) large systems. The objective of this paper is to further develop and exploit the idea of combining a formal approach on the agent level and an empirical approach on the system level in self-organisation.

INTRODUCTION

The self-organising 'paradigm' is the response to the increasing need for systems that are adaptive, flexible and pliable towards uncertain operations of the units that build it up and the interactions between these units. These new computational systems (also known as pervasive technology or emergence engineering) consist of many (in order of thousands) units exhibiting complex behaviours on different aggregation levels. The aggregation levels vary from local (micro) behaviour on the unit level to global (macro) behaviour on the system N. Ferreira-Schut Department of Computer Science Radboud University, Nijmegen (NL) nivea@cs.ru.nl



Figure 1: The design problem, with 3 agents who have to find a good mapping between their inputs (black circles) and outputs (white circles).

level. Real-world examples of such systems are abundant: traffic networks, energy distribution networks, markets, computer networks, animal and human societies.

The problem addressed in this paper concerns the *design* of self-organising systems. Consider Figure 1 as an illustration of the self-organising system design problem: a homogeneous set of agents in which each agent receives an input (i.e., observes) and generates output (i.e., acts), and faces the problem of mapping its received input to a 'good' output. Although it is extremely general and simple, this illustration captures a very wide range of applications, including, for example, protocol design for very large computer networks, design of collective robotics and inter-vehicular communication for automative traffic engineering.

Throughout the paper, we define *self-organisation* in a strong way: a system is self-organising if, and only if, there are no organisational roles allocated to the system's parts (i.e., agents, individuals, elements). This definition excludes systems in which (designed or emerged) organisational roles exist, for example, managers, brokers, superiors or subordinates (which would be weakly self-organising). Different individuals can still be *specialised* in a functional way (related to the system's task), but not in an organisational way. The main argument for this approach is that we want to know the true power of self-organisation by leaving out organisational structures and to keep the agents as simple as possible – making it possible for the intelligence to emerge at the system level instead of at the agent level.

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) The current state-of-the-art regarding the design problem is that there are in general 3 widely-used approaches: 1) simulation – construction of a simulation model followed by statistical analysis, 2) formal – building a formal model of the problem/solution and checking whether desired properties do hold or not; and 3) nature-inspired – taking observed methods and techniques from nature as the starting point (e.g., ant foraging, honeybee dancing, see (Camazine et al. 2001)) and 'finding' problems that can be solved with these methods and techniques.

We consider none of the above described approaches absolutely ideal to be used as a 'generic' design framework. For simulation, the major drawback is that the modeller has no means to verify the local workings of the system - the observed and analysed results are on the system level and not on the agent (individual) level. With a formal approach, it is only possible to look at 'small' systems because of the computational complexity of these approaches. A weakness of the nature-inspired approach is that it is not a 'problem-centered' one (instead, it is a reverse engineering approach, see (Zambonelli et al. 2005)). Also, all approaches are developed ad-hoc within the context of a given problem or domain. To date, there has been no successful attempt to develop a generic design framework with the explicit aim to be useful for a wide range of application problems.

The research objective of this paper is to further develop and exploit the idea of combining a formal approach on a local level and an empirical approach on a global level in self-organisation.

Although this paper is (only) a very first step towards the long-term aim of delivering a generic framework, we can clearly identify the originality of the proposed research: 1) it deals with design limitations of nature-inspired (reverse-engineering) approaches (e.g., swarm intelligence, see (Bonabeau et al. 1999)), 2) it does not exclusively focus on either formal or simulation approaches, and 3) it introduces self-organising systems as an interesting new system class for existing modelling techniques (e.g., Markov decision processes, as described below).

RELATED WORK

Design of Self-Organisation Although there is a general trend and steep increase of interest in the design of self-organising systems, there is only a handful of related research specifically aimed at the *domain-independent* (or: general) design of self-organisation. We briefly enumerate this work here in order to sketch a context for our paper. Note that we did not include here: work that looks at the "emergence problem" (the relation between the local and global levels in a self-organising complex system) (de Wolf and Holvoet 2005), because we consider it best to investigate this after successful application of the proposed framework, enabling us to systematically examine this problem; work where individual agents in a self-organising system have or develop organisational

roles, because these systems do not fit the strong notion of self-organisation used in this paper; and work that is strongly theoretical, e.g., (Yamins 2007).

We briefly sketch the history of design approaches in the last decade. In 2003, (Serugendo 2003) sketches the idea of engineering emergent behaviour and in subsequent work identifies comparison criteria for selforganising systems, categorises mechanisms leading to self-organisation, and proposes an approach for selecting self-organising mechanisms. In 2004, (Edmonds and Bryson 2004) use the experimental method as the starting point of an adaptive strategy for producing self-organised software. In 2005, (Bar-Yam 2005) proposes multiscale analysis as a way to engineer complex systems; (Wolf and Holvoet 2007) categorise design patterns for decentralised coordination in self-organising systems. (Gershenson 2007) proposes a design methodology based on the idea that reducing the 'friction' of interactions between elements of a system will result in a higher 'satisfaction' of the system. In 2007, (Sudeikat and Renz 2007) suggest to use the approach of requirements engineering to develop self-organising multi-agent systems. And last year, (Martinoli 2008) proposes the use of multilevel modelling to design swarm (robotic) systems; also, (Gardelli et al. 2008) propose a simulation-driven approach to design self-organising environments.

The most important difference between the research in this literature overview and the work suggested in this paper is exactly the novelty of our work. Although, as shown above, some references also make the formal/empirical distinction, nowhere is it combined with the individual/system level. For instance, a state of the designed system is represented on the global level (all individual nodes are within one state), while we propose to do this only on the local level (i.e., individual-centered) and clone the agent to lift it to the global level (and then investigate the system empirically).

Multi-Agent Systems We understand that selforganising systems demonstrate complex behaviour even if their individuals are decribed in terms of simple strategies and knowledge - though some aspects of more common 'intelligent' multi-agent systems, see (Wooldridge 2002), such as autonomy, decentralisation and local view are still present. In terms of multi-agent systems, our research restricts its interests by considering a self-organising system as a collection of interactive individuals, which are uncomplicated, basic, light-weight in their specification. Opposite to this, being intelligent means that the agent is capable to reason about the world given the information it obtains and following its behaviour description. Our interest lies in stochastic systems in which the options of actions that such a reasoner can take follows a probabilistic distribution. Additionally, reward functions are used to allow the specification of strategic mechanisms, i.e., based on these functions, an agent will endeavour on establishing the best set of actions that leads to its goal(s).

Markov Decision Processes Our first attempt at a formalisation of the local level will be by means of a Markov decision process, hence a brief introduction. In general, a Markov chain, according to (Baier and Katoen 2008), is a directed graph where nodes represent (system) states and relations among those states are captured by probabilistic transitions. Markov decision processes (MDPs), see (Bellman 1957), extend Markov chain by the explicit represention of actions which generate the transitions among states. One can use an MDP in order to model problems in which the decision making process in uncertain environments is automated. By uncertain environments we mean that the outcomes of actions are not entirely predictable. By automation we mean that we can use algorithms in order to 'solve' an MDP (i.e., derive a policy which maps states to best actions).

Well-known exensions of the 'basic' MDP model that are relevant to this paper are partially observable MPDs (or: POMDPs, see (Kaelbling et al. 1998)) and multiagent MDPs (or: MMDPs). Regarding the latter, (Jamroga 2008) presents a formal language, MTL, which allows the representation of general scenarios in which a system is formed by multiple agents (or: processes) which interact to one another. In this case, sets of agents can establish joint strategies in order to achieve (common) objective(s). A model for the multi-agent MTL is a refinement of MMDPs, see (Boutilier 1999). The main difference with the work by Jamroga is that Boutilier focus on fully cooperative multi-agent systems, while the former allows the specification of sets of agents that might not share the same objectives - accounting, therefore, for more general scenarios. Still, in both, agents are assumed to know the global state of the system at all times. Another approach also related to Boutiliers and to multi-agent MDPs is the framework proposed by (Xuan et al. 2000). This approach also concentrates on the description of fully cooperative systems. But here the decentralised aspect of multi-agents systems is emphasized. Instead of assuming the omniscience of agents, decentralised control of finite state Markov processes is used.

For us it is clear that formalisations of MDPs such as presented by (Jamroga 2008) is highly relevant. First, we can represent agents using a MDP model and specify properties regarding the behaviour of those agents. Then, we are able to verify whether those desired, or required, properties in fact hold.

In the next section we present our framework, establishing in more detail the role of specification and verification in our self-organising design.

SOLUTION FRAMEWORK

The solution that we propose is a design framework (shown in Figure 2) based on the before-mentioned simple idea to approach the agent level formally and the system level by means of simulation. This synthetic approach allows us to do rigorous formal verification of the behaviour of the individual agents as well as large-



Figure 2: The proposed solution framework.

scale empirical validation of the system as a whole. It also exploits the specific advantages of the approaches regarding the scale of the system: formalisation is good for small systems while simulation works well for (very) large systems. Thus, differently from other approaches, we do not attempt to either fully formally *specify* the system behaviour, nor do we blindly rely on observed system behaviour while not knowing what happens at the local level.

The reason that this approach potentially works well for self-organising system design (but possibly not for system design in general) has to do with two important aspects of a self-organisation itself. Firstly, although such systems are massive (i.e., involve many agents), they are formed by homogeneous set of agents (e.g., bird flocks and fish schools). This property makes the modelling and designing of these systems somewhat easier than 'complicated' systems - especially concerning the representation of the agents and, subsequently, scaling up the system (almost by simple 'cloning'). Secondly, the interaction among the agents occurs 'only' with their direct neighbours. Thus there is no need (not even theoretically) to consider the possibility that two distant agents interact with each other. Also, the nature of the interaction differs from cooperation in the traditional sense agents rather *react* to each other (like birds in flock on the basis of separation, alignment and cohesion).

Our framework consists of 4 subsequent development phases, i.e., formal specification, verification, simulation model and validation. The arrows in the Figure 2 indicate how the phases relate to one another. Note that a special case of such general description is having a system that goes successfully from specification to validation, never returning to a previous phase.

Formal specification As previously mentioned, we understand an agent to be an autonomous entity capable of observing (or *partially modelling*) the world (i.e., the domain in which it is situated) and acting in accordance with those observations. In order to obtain an accurate agent description, a diversity of languages adequate for an agent specification have been produced. In this context, logical languagues are characterised by their unambiguous semantics, and have been applied as useful formalisms for agents' description, allowing also agents' implementation and verification, see (Fisher et al. 2006; Barringer et al. 1996). In other words, logical formalisation of agent behaviour is desirable, not only in order to provide a clear semantics of agent-based systems, but

also to provide the foundation for sophisticated reasoning techniques. For these reasons, we opt for applying a formal language for the representation of agents in this step of the design of self-organising systems.

Verification Well-defined syntax and unambiguous semantics of a formal language allow an accurate agent description to be produced, while also potentially allowing formal verification tools to be applied. Logical verification can (and should) be used in order to guarantee that malicious behaviour of individuals are avoided, something that is of crucial importance in complex and critical applications. In this phase of the system's design, we aim to verify that certain (desired) properties regarding individual behaviour are guaranteed, before proceeding to the system simulation where the self-organisation aspect (and, consequently, broader scope) comes into play. A method for formal verification of (agent-based) systems is model-checking, see (Baier and Katoen 2008). Essentially, this method performs an exhaustive search through a finite-state specification aiming to obtain a way in which the required property might be contradicted. In model-checking an agent is given in terms of local states in some structure.

Simulation model The simulation phase is the first one on the global level of the system design. It is through the simulation process that a system's emergent behaviour can be produced. That is, in our simulation phase a model is obtained in which a large number of individuals is considered, and as a result of their interaction the selforganising aspect of the system can be generated. For example, consider an artificial society in which the task of individual agents is solely to survive on the basis of collected resources that exist in the environment. The model that you use for this simulation can be a simple rule-set to be executed by an agent: each agent is a rule-based system. If the agents are able to learn, an adaptive algorithm is added to the simulation in order to make such learning possible. The simulation then adds the control loop to the whole system (model + algorithm) and allows you to switch on the model and observe its development over time. In short, it is through simulation that the real scale of the system can be achieved. It is only in such dimensionality that the emergent intelligent behaviour of the society can finally be accomplished and analysed.

Validation Validation of a self-organising system refers to the conclusions that can be drawn for the system behaviour, observed during the simulation phase. In this context, some statistical methods, such as two-sample t-test and analysis of variance, allow the interpretation and evaluation of *emergent* behaviour. In this sense, emergent means that "the whole is more than the sum of the parts" according to (Damper 2000). In other words, emergents – which are novel with respect to the individual parts of the system – arise dynamically from

the interaction among those parts, following (Wolf and Holvoet 2007). Other criteria (or: 'a properties) can be checked (besides general properties of self-organisation, see (Holland 1995)): *robustness* – capability of the system to remain operational in the face of (unpredicted) variations of the environment; *adaptivity* – which refers to the quality of fitting to given changes in the environment; in our context, an individual might change itself or the system as a whole might change; *redundancy* – when knowledge or information is kept in different locations of the system; and, *success* on the completion of required application task(s).

SPECIFICATION WITH MDP

We investigate whether the MDP model is an appropriate one for the formal specification in our proposed solution framework. Here, we define an MDP following (Jamroga 2008),

Definition A Markov decision process over domain $D = \langle U, \top, \bot, - \rangle$ and a set of utility symbols Π is a tuple $M = \langle S, Act, Pr, \pi \rangle$, where

- S is a finite and non-empty set of states;
- Act is a non-empty set of actions;
- $Pr: S \times Act \times S \rightarrow [0,1]$ is a stochastic transition relation and $Pr(s_1, \alpha, s_2)$ defines a probability with which the system will go to state s_2 , if it is in state s_1 and the agent performs action α . Being a probability distribution, for each state $s_1 \in S$, $\sum_{s_2 \in S} Pr(s_1, \alpha, s_2) = 1$, or $Pr(s_1, \alpha, s_2) = 0$ for all s_2 , in case α is not enabled in s_1 .
- $\pi: \Pi \times S \to \hat{U}$ is a valuation of a utility *fluent*.

The definition includes that a utility and/or propositional symbol (referred to as fluents) can be assigned to each state of the Markov decision process model. The domain consists of a set of utility values $U \in \mathbb{R}$, \top and \bot representing the logical truth and falsity, and \neg the complement function. Besides, $\hat{U} = U \cup \{\top, \bot\}$. In this context, a policy can then be defined as a sequence of steps which specify the set of (future) actions to be taken by the agent. In such context, policies can also be stochastic. In short, Markov decision processes define stochastic systems which involve strategic reasoning, decision making and reward/utility functions.

In the next section we present an example of selforganising system in which all phases of our framework is described, and MDP is the underlying model for an agent representation.

EXAMPLE

We consider here a short example to illustrate the ideas presented above. The example concerns a simple game. Assume that we have a $x \times y$ checkers board with in total *i* black and *j* white pucks. The pucks are scattered randomly over the board. On the board are also k robots situated that have to collect the pucks. Each agent also has a colour, black or white, and can only pick up pucks of the same colour as itself. An agent can observe pucks and other agents on the m surrounding cells; move horizontally (East, West) and vertically (North, South); it can pick up pucks, and also change colour. The aim of the game is for the group of agents as a whole to converge on a division of labour where the ratio for black/white robots is equal to the ratio of black/white pucks. Here, we are interested in the *with-replacement* version of the game: when a puck has been picked up by an agent, it is put back on the board at another random empty cell. (In the without-replacement version, an alternative aim of the game is to pick up all pucks as fast as possible.) We have not implemented the example in a computer model, but here we do give a preliminary outline of the different steps in the introduced framework.

Formal specification

Based on the general MDP definition given above, we formalise the agent states and actions as well as the reward function from our example. We let the state of an agent be a vector containing 1) its own colour, 2) the colour of the puck that the agent currently stands on (has value 0 is the agent does not stand on a puck), 3) the number of black agents, 4) the number of white agents, 5) the number of black pucks, and 6) the number of white pucks in the agent's neighbourhood. The agent receives a reward r when it picks up the puck that it currently stands on, it 'pays' a penalty c when it changes colour. Besides, the absolute value of r is much higher than the value of c.

 $\begin{aligned} Agents &= \{1, \dots, k\}, Colour = \{b, w\};\\ St_i &= \langle col_i, puck_i, \#ag_b, \#ag_w, \#pu_b, \#pu_w \rangle,\\ where \ i \in Agents, \ col_i \in Colour,\\ puck_i \in Colour \cup \{0\},\\ ag_{colour} &= [colour] \ agent,\\ \#ag_{colour} &= number \ of \ agents \ in \ neighbourhood,\\ pu_{colour} &= [colour] \ puck, \ and\\ \#pu_{colour} &= number \ of \ pucks \ in \ neighbourhood;\\ Act &= \{N, S, E, W, PickUp, ChangeColour\};\\ Reward (\langle b, ..., .., b \rangle, PickUp) &= r,\\ Reward(\langle b, ..., .., .., \rangle, ChangeColour) &= c,\\ where \ _is \ a \ wildcard, \ r \ and \ c \ are \ constants,\\ r &> 0, c < 0, \ and \ | \ r \mid \gg \mid c \mid. \end{aligned}$

In the example, the transition function represents moving from one neighbourhood state to another. In the formalisation above, we opted for a very concise description of the state, making the role of the transition function somewhat more important. More detailed state descriptions can also be considered that could include information about the distance to the other robots/pucks or even the exact location relative to the agent's own location. With respect to a suitable action policy, i.e., a sequence of actions to the taken at each state in order to maximise an agent's reward, either an automated or hadmade policy can be established. This means that either MDP solution algorithms (e.g., value/policy iteration) can be applied in order to obtain a system's solution, or a 'hard-coded' solution can be described.

Verification

Given the nature of self-organising systems, we do not have a notion of global states (i.e., representing the state of all the agents). Therefore, the described properties do not refer to group objectives or team performance which should be optimised. Instead, we define and verify properties that only refer to an agent's individual behaviour or aim. For instance, we may be interested in verifying whether it holds that "an agent *eventually* collects a puck". Moreover, and perhaps more interesting, is a property which establishes that "an agent picks up as many pucks as possible with the least possible colour changes".

Although we are aware that properties regarding the behaviour of small groups of agents can also be verified, due to the scale of self-organising systems (as mentioned above), only through simulation the full behaviour of the system can be observed and further analysed. An example of such a (small group) property is whether it is guaranteed that "the ratio of the number of black/white pucks is the same as the ratio of the black/white agents".

In order to specify and verify such system properties, a suitable logical language is needed. The language proposed by (Jamroga 2008) could be considered as a potential formalism for this purpose. However, it still remains to be evaluated in detail how its description fits to the our concept of multi-agency in self-organising systems. For instance, we might require a more generic description of a system - more closely related to the concepts of POMDP. This should allow us to avoid the usual requirement of knowing the global state of the system.

Simulation model

The purpose of the simulation model is to obtain information about the global level of the system. In other words, for our example, we are interested to see if all agents together can achieve convergence towards equal black/white robot and puck ratios. As mentioned above, the generic approach to constructing the simulation model is to take the individual agent model as specified formally and 'clone' it to scale it up to reach a typical self organisational system size. We expect the formal specifications to be as such that the step towards implementation (and produce software) is as small as possible. Besides this 'cloning' process, we need to take some design decisions on the environment in which the system is situated. In the example, we need to define the size $(x \times y)$ of the board. With the simulation model being complete, we need to design and set up the experimental parts of the simulation. Thus, we have to define *independent* and *dependent* variables as well as *contingency* (exogenous) variables. Typically, in these kinds of simulation experiments, there are many of such parameters and we must carefully craft the experimental design to restrict ourselves in terms of what we want to investigate. The objective(s) of the study should work as restrictors here. In this puck-collection study, we can vary, for example, the number of robots, number of pucks, or size of the board. Then we can measure the effect of these variables on, for example, the black/white robot and puck ratios, or the total number of collected pucks. Also, if we have specified a number of different control policies for the agents, we can test the performance of those policies in comparison to each other.

Validation

The properties to be *validated* on the global level have the form of statistical hypotheses: statements on correlations between independent and dependent variables in the experimental design/setup. In our example, the most important hypothesis concerns two dependent variables: the ratio of the number of black/white pucks, and the ratio of the black/white agents. It depends on our particular interest how we are going to investigate this (regarding a suitable hypothesis), e.g., do we want to show this in general, only for particular board sizes, only for particular numbers of robots or pucks?

In general, whereas the logical verification of the individual level concerns checking correctness, i.e., "does my agent do what I expect/want it to do?", the properties on the system level generally concern performance criteria, i.e., "is the collection of agents effective with respect to some shared goal or objective?". Besides such (domain-dependent) performance criteria, we already mentioned the apparent useful (generic) properties of self-organisation: robustness, adaptivity and redundancy. Testing these in terms of statistical hypotheses means that these properties must, first of all, be quantified and then included in the (in)dependent variables. Robustness and redundancy are related to size of the system (number of agents) and the flow of information between agents; adaptivity can be 1) hardwired into the agents themselves (and is thus not testable), 2) measured on the local level (an individual agent adapts to changing circumstances), or 3) measured on the global level (individual behaviour is not adaptive, but the system as a whole is, i.e., like a flock of birds.

Finally, note that we do not aim to 'solve' or explicitly acquire further knowledge on the before-mentioned "emergence problem". In our experience (and also observed by others), attempts to investigate this problem either exclusively formal or empirical are prone to failure because of the system size (formal approaches do not scale) or individual behaviour/interaction (simulation loses touch with the local level). As mentioned, we are mainly interested in the resultant outcome of the system, without necessarily finding out more about 'emergence' as a phenomenon.

CONCLUSIONS

We have seen that nature can bring us useful methods and techniques, but it seems that the range of applicability is limited: we know of a small number of problems that can be solved – travelling salesman problem, dynamic routing, collective robotics – but we may have hit the boundaries. It is time to change our frame of mind: instead of the *solution-centered* way of approaching self-organising system design (i.e., we have a solution provided by nature and find a problem that we can solve with it), we need to move to a *problem-centered* approach in which there is a problem to be solved and we can use a (generic) design framework to pour the problem in and systematically investigate potential solutions.

In terms of developing such a framework, we need to 1) *conceptualise* the problem class (to know what we are talking about), and to 2) *formalise* the problem/solution space (to see if solutions can be found) – eventually leading up to an *operational* framework containing design principles and/or solution algorithms. However ambitious the ultimate goal is to create such a framework, it would meet the challenge set to the community: *to develop applications that "work for themselves" – define a global goal, design components and local functionality and check that the desired result will emerge during execution, as coined by (Serugendo 2003).*

This paper is a small step in between steps 1 and 2 in the above described timeline. We have started with the conceptualisation in earlier work (outlined in (Schut 2007)) and are now exploring ways to put the conceptualisation on a more formal footing. As such, we do not aim to deliver a framework that will generate a solution – i.e., solve the mapping problem for the individual agents in the above-mentioned design problem (Figure 1). Instead, what we aim to achieve is a framework in which we can 1) represent a design problem, and 2) systematically examine potential solutions by effectively integrating formalisation and simulation. A possible next step after successfully examining potential solutions systematically, further automation applied to the framework could potentially involve generating solutions.

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MACSIMA: AN AGENT FRAMEWORK FOR SIMULATING THE EVOLUTION OF NEGOTIATION STRATEGIES IN B2B-NETWORKED ECONOMIES

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KEYWORDS

Agent-based Simulation and Modeling, Agent-based Supply Chain Management, Learning Agents, Supply Networks, Coordination Mechanism Design, Bilateral Negotiation, Genetic Algorithms, Output Analysis.

ABSTRACT

In this paper, we describe the multiagent supply chain simulation framework MACSIMA. This framework allows the design of large-scale supply network topologies consisting of a multitude of autonomous agents representing the companies in the supply network and acting on their behalf. MACSIMA provides all agents with negotiation and learning capabilities so that the co-evolution and adaptation of the price negotiation strategies of the business agents that exchange goods over an electronic business-to-business (B2B) market can be simulated and evaluated. An electronic B2B market is a market run by computers (and often mounted on a website) providing facilities for companies acting as suppliers to post offered materials, products, services together with price ideas on the market and matching these offers with the demand of other companies acting as producers or retailers. Thereby MACSIMA supports a fine-tuning of the parameterization of the learning mechanism of each individual business agent and additionally enables the agents to exchange information about finished negotiations with other cooperating agents. We outline evaluation results with a first focus on the emergence of niche strategies within a group of cooperating agents. After that we center a second focus on the coordination efficiency, i.e. on the effects of the application different of learning mechanism parameterizations on the overall turnover and profit of supply networks. Our simulation results show that depending on the parameter setting of the learning mechanism the outcome (e.g. the overall turnover) of such a supply network can vary significantly.

INTRODUCTION

A *supply chain* is a chain of possibly autonomous business entities that collectively procure, manufacture and distribute certain products. Since today's markets are highly dynamic, supply chain partner companies are forced to form supply chains on the basis of more

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flexible and co-operative partnerships. For these reasons, so-called supply webs (Laseter 1998) (Porter 2000) - i.e. dynamic networks of supply chain units enabled by B2B markets - will replace today's static supply chains to an increasing extent. In such B2B-enabled dynamic supply networks, the selection of partner companies producing and supplying needed resources and semi-finished goods is not fixed in advance but is carried out over electronic markets through instantiated coordination mechanisms, e.g. specialized auction or negotiation mechanisms, according to the current state of demand. This means that due to their dependence on the changing environment, the members as well as the topology of the supply network are constantly evolving. But taking part in such specialized B2B coordination mechanisms increases transaction cost and can get too complex for humans to handle efficiently. In order to cope with this dilemma it is suggested by numerous researchers to encapsulate operative supply chain units within agents (Chaib-draa and Müller 2006) that are able to adapt themselves to varying circumstances and partner companies quickly and efficiently. Agents offer the advantage of being able to automatically form and manage such changing partnerships since they can autonomously perform tasks on behalf of their users and in doing so reduce transaction cost.

But so far there exist almost no consolidated findings about what coordination efficiency results if negotiations about the exchange of goods in a large-scale B2B scenario are totally transferred to business agents that are purely self-interested and thus do not strive for mutually beneficial transactions but try to outperform their partners by elaborated negotiation strategies. To examine the resulting dynamics within a supply network built up by adaptively negotiating agents, we have instantiated MACSIMA (<u>Multi Agent Supply Chain SIMulAtion</u> Framework).

THE MACSIMA FRAMEWORK

The MACSIMA framework has been implemented in Java and offers a set of generic supply chain agent types for instantiating supply network scenarios with the ability to take part in bilateral negotiations, as well as with elaborated learning capabilities, enabling them to learn from negotiation successes and failures in order to adapt their negotiation strategy iteratively.

Generic Agent Types

The generic supply chain agent types provided by MACSIMA are

- 1. *resource or supplier agents* (R_i) supply raw materials to the network.
- 2. *producer agents (Pi)* stand in the middle of the value chain and buy raw materials or semi-finished goods from resource agents or other producer agents as input goods to their production function and offer their output goods for purchase.
- 3. *consumer agents (Ci)* stand at the end of the added value network and buy products from the producers. They cannot run out of money, but however, have a consumption function that specifies their maximal willingness to pay.
- 4. *good agents (Gi)* keep an account of the number of successful (transactions) or unsuccessful (rejections) price negotiations concerning a specific good together with the negotiated prices etc. These agents are not necessary for conducting simulation runs but simplify the statistical evaluation of simulation results.

In MACSIMA, simulation scenarios can be defined and parameterized in a very detailed way as well as with a high degree of freedom, so that the user is totally free to decide on the number of tiers and interacting agents.

Simulation Scenarios and Building Blocks

In our simulation runs conducted so far we have concentrated on different instantiations of a five-tiersupply-network for computer manufacturing (see fig. 1).



Figure 1: Scenario for Computer Manufacturing

MACSIMA makes it possible to define scenarios with very complex and voluminous topology graphs by combining generic supply web building blocks (fig. 2).

Therefore, MACSIMA offers a graphical user interface that not only simplifies the definition of topologies but also enables one to parameterize the learning capabilities of <u>each</u> agent that is instantiated for a simulation run in detail as described later. The instantiated agents find each other by a directory service that administrates all the agents within a simulation scenario with their *unique* names, addresses, agent type and properties, i.e. capabilities, offered and demanded goods etc.



Figure 2: Example for Supply Network Building Blocks

Supply agents use this directory to find other agents with possibly intersecting goals, i.e. who offer desired goods or who are looking for desired goods. To find out if a mutually beneficial transaction can be carried out, each agent may select another agent in the network for starting a bilateral negotiation. The control cycle of a MACSIMA producer agent is sketched in figure 3. If an agent is instantiated as a supplier or consumer agent, the control cycle is shortened by turning some functions, e.g. *Start Buy-Negotiation*, off.



Figure 3: Control Cycle of a MACSIMA Agent

We usually run scenarios with 25 to 100 agents on an Intel Quadcore-architecture with 3 GB RAM and 32bit Windows Vista as operating system.

Negotiation Protocol

In the bilateral negotiation process, all agents are provided with the same action alternatives derived from Pruitt's *strategic choice model* (Pruitt 1981).

Negotiation Acts

This model states that humans show specific behavior in economic negotiation scenarios and select in every negotiation round from among five basic strategies, namely

- 1. *unilateral concession*: decreasing the distance between conflicting positions,
- competitive behavior: remaining with one's position and trying to argue the other party out of its position,
- 3. coordinative behavior,
- 4. *idleness*: not continuing the negotiation, or
- 5. *demolition*: withdrawing unilaterally.

(Eymann 2000) states that these basic building blocks can be reduced to three *negotiation action alternatives*:

- 1. *Accept*: the price proposal of the other agent is accepted and the transaction is conducted. The buyer pays the end price to the seller and receives the product.
- 2. *Propose*: the agent at turn does not agree to the price proposal of its opponent and makes a new proposal on its part. This new proposal can be equal to its last proposal (no concession in this round of negotiation) or be newly calculated.
- 3. *Reject*: an agent breaks off the negotiation. Both agents thus have to search for other negotiation partners.

On the basis of these three negotiation acts the agents in MACSIMA use the following negotiation protocol that is sufficient for modeling bilateral price negotiations between agents in the examined supply network application domain.



Figure 4: Bilateral Price Negotiation Protocol

Strategy Parameters

For modeling complex strategic negotiation behaviour on the basis of the described action alternatives we use six *strategy parameters* that determine the negotiation strategy of an agent. These can take on values from the interval [0;1] and are stored in a so-called *genotype*, a data structure suitable for processing by a genetic algorithm:

- 1. acquisitiveness (A)
- 2. delta_change (DC)
- 3. delta_jump (DJ)
- *4. satisfaction* (*S*)
- 5. weight_memory (WM)
- 6. reputation (R)

An agent possesses several genotypes – i.e. vectors of the form $\langle A|DC|DJ|S|WM|R \rangle \rangle$ containing these parameters – that are stored in its *pool of genotypes* (see figure 5, right upper corner) and are evolutionary adapted to varying negotiation partners and market conditions as described in figure 5 and the section "Negotiation Module". Each parameter of a genotype influences non-deterministically an agent's individual negotiation behaviour.

The *acquisitiveness* of an agent defines the probability that it will offer a unilateral concession on its next "move", i.e. as the seller lowering its asking price. This

parameter taking on a value of 1 would prohibit an agent from making any price concession.

The *delta_change* parameter defines the step size of a monetary concession by specifying a percent value by which the price distance between one's last price proposal and the counter offer of an opponent is reduced. An agent calculates its *individual* step size for a concession at the beginning of a negotiation by using

This keeps the negotiation mechanism *symmetric* since neither sellers nor buyers are handled in a preferred manner (for attributes of a coordination mechanism see (Fischer et al.1998)).

The *delta_jump* parameter defines the margin an agent wants to realize. The higher its value, the higher the aimed margin between the buying costs for input goods and the demanded selling price will be. *delta_jump* modifies the first price proposal of agent A by:

$$proposal = agreement * (1.0 + del_jump)$$

where *agreement* equals the price of the last deal for the good.

The parameter *satisfaction* defines the probability that an agent aborts the negotiation. The abort probability after the nth negotiation round is $(1 - p_satisfaction)^n$.

To avoid individually nonsensical behaviour the agents have a learning function to detect unreasonable price proposals during a negotiation. Therefore an agent stores the end prices of successful negotiations from its negotiation history in a data structure *memory* and calculates an internally "*sensed*" *market price* (*SMP*) for each good of interest. The information stored in *memory* is used to compute its *smp* with exponential smoothing. Thereby, the parameter *weight_memory* specifes how fast market changes have influence on the market price.

// update our memory of initial prices
memory = offeredPrice * weight_memory
* (l

+ memory * (1-weight_memory);

On this basis, at negotiation start each agent checks the first price proposal of its opponent against its SMP. All counter-proposals lying between the SMP and its doubled value are estimated as uncertain and a possible negotiation abort is tested according to *p_satisfaction*:

All counter-proposals exceeding the doubled SMP are directly rejected to avoid extortion offers. The last parameter *reputation*, defines the probability of finishing a deal correctly according to the reputation of a partner. The values of these six parameters describe completely the negotiation behaviour and are adapted by the agents' negotiation module during a sequence of negotiations.

Negotiation Module

Each negotiation module of an agent possesses a *genetic pool* of genotypes. This pool contains several genotypes that are employed in negotiations. After a negotiation has been finished a *fitness value* is calculated for the genotype in depending on the negotiation outcome. Then the genotype is stored in combination with the ascertained fitness value as *plumage* in a data structure called *population*. The sizes of pool and population can be flexibly set for the negotiation module of each agent.

After the start of a bilateral negotiation, the first step of an agent is to choose a genotype - determining its strategy for this negotiation - out of its pool of genotypes. Then, both agents negotiate until one of them aborts the negotiations or their price proposals cross and they make a mutually beneficial deal. After a successful negotiation both agents calculate a fitness value for the used genotype and store the resulting combination of genotype and estimated fitness as a so-called plumage into the population data structure.

If their information exchange mode is set to external or mixed, they will afterwards send the resulting plumage to other agents, receive plumages from other allied agents and store the self-calculated as well as the received plumages in their population. If the number of stored plumages is larger than the population size the agents will start their learning process by using their individually parameterized evolutionary learning mechanism as sketched in figure 5.



Figure 5: Co-action of Negotiation and Learn Process

Parameterization of the Learn Process

When the learning process is started all plumages within the population are assigned to a *selection method*, which selects the plumages with the best fitness values and assigns as many plumages to a *recombination process* as the pool size allows. In this recombination process selected genotypes are recombined to new genotypes. Optionally, the newly built genotypes can be modified by probabilistic *mutation* after the recombination. In the last step, the old population of the agent is deleted and the newly generated pool is assigned to the agent according to its specific replacement scheme. After that the agent may start new negotiations. The possible settings for information exchange and the parameterization of the learning process are described in the following.

Information Exchange

An agent learns either only by itself (*internal learning mode*), i.e. does not use the experiences (in the form of plumages) of other agents. Or an agent has "colleagues" that exchange plumages about successful finished negotiations and use this information in their next evolution step (*external learning mode*).

Fitness Calculation

After a successfully finished negotiation, i.e. a mutually closed deal, the fitness value for the genotype used in the negotiation is calculated. MACSIMA offers the agents' designer the following *fitness calculation methods:*

1. The *price_minus_average (PMA)* fitness function uses the margin between the current average price of a good and the current price:

2. The *percental_average_proceeds* (*PAP*) method takes the duration of a negotiation into account by dividing the PMA fitness value by the average price times the number of rounds in which this genotype was used.

$$fitness = \frac{average \Pr ice - current \Pr ice}{average \Pr ice * rounds For Gurrent Genatype}$$

3. The *percental_absolute_proceeds* (*PAB*) method divides the value of the PMA variant by a fixed basicPrice times roundForCurrentGenotype.

$$fitness = \frac{basic \Pr{ice} - current \Pr{ice}}{basic \Pr{ice} * roundsfor CurrentGenotype}$$

4. The *percental_mean_proceeds (PMP)* method uses the mean value (mediumPrice) of the starting price proposals of both partners in the negotiation.

$$fitness = \frac{medium\Pr{ice-current}\Pr{ice}}{medium\Pr{ice*rounds}ForGurrentGenatype}}$$

Selection

- 1. *Binary competition (BC)*: Two randomly selected individuals are compared and the one with the higher fitness value is selected and copied in the new population. This is done repeatedly until the new population has reached its defined maximum size.
- 2. *Roulette-Wheel-Selection (RWS)*: Each individual I is assigned a section on a wheel based on its fitness value according to the formula:

$$\alpha = 360 \frac{f(I_k)}{\sum_{n=1}^{N} f(I_n)}$$
, with

 α = Angel assigned to the kth individual, $f(I_K)$ = Fitness of the kth individual and N = Number of individuals.

3. *Deterministic Selection (DS)*: Based on the fitness value of the individual i an expectation value is calculated:

Expectation
$$E(X) = f_i \frac{N}{\sum_{k=1}^{N} f_k}$$

- 4. Deterministic Average Selection (DtS): In the case that the same genotype has been used in several negotiations and thus is contained in the population more than once this method calculates the average fitness value for each individual genotype before the selection starts. The individual with the best fitness value comes directly into the new population; the worst one is deleted and the remaining genotypes are selected as in the DS method.
- 5. Deterministic Average Selection with deletion of the worst individual (DAS): The new population is filled up in the same way as with the standard deterministic average selection until the number of individuals in the new population equals pool size minus the value of *BestIndividualsToSurvive*. For the last place a new genotype is generated as the mean value of each gene of the genotypes already in the new population.

Recombination

This crossover of individuals with good fitness values is a kind of macro mutation which creates jumps in the search space and therefore helps to find a better solution.

- 1. *n- Point- Crossover (nPC)*: The two best individuals are taken out and with a *crossover probability*. These two are recombined and cut at 'n' randomly chosen positions and linked crossover or they are put back in the population unchanged. The new generated genotypes replace their parents in the population.
- 2. *Random Crossover (RaC)*: Two individuals are selected and for each gene it is decided randomly if it is taken for the new genotype.

Mutation and Replacement Scheme

Its main target is to keep the diversity in the population. Usual modifications are implemented in MACSIMA as suggested in (Back et al. 1997).

Simply deleting the old pool bears a risk that all new genotypes are worse than their parents. To protect the best individuals MACSIMA provides the replacement schemes *Elitism and Weak Elitism* (Back et al. 1997).

Differentiation Factors of MACSIMA

An advantage of MACSIMA is the ability to set up nearly all possible supply network layouts and to instantiate them with numerous intelligent agents using a *learning mechanism* that can be adjusted to great detail.

The experimental results of (Lau et al. 2006) show that such an evolutionary learning approach for adaptive negotiation agents in e-business scenarios can outperform a theoretically optimal negotiation mechanism guaranteeing Pareto optimality.

This is a progressive step as compared to the limited learning features of precedent approaches for the simulation and analysis of the effects of learning on the outcome of negotiations in such environments. They offer only very limited learning capabilities, e.g. (Eymann 2000) and (Smith and Taylor 1998), and almost no support in examining the effects on the generation of social welfare quantitatively. One further differentiating factor consists in the fact that MACSIMA agents can use different information exchange modes with respect to the extent of information exchange with other agents. In this way, the experimenter is able to build cooperating groups out of several agents on each tier and to examine the effects of coalition formation between agents. In this way, the evolution of an agent's negotiation strategy is not only guided by its own experience but can also take the experience of other agents into account.

Both allows for comparing different learning mechanisms in combination with different information exchange modes under the same external influences and constraints in a supply network. To our knowledge MACSIMA represents so far the only simulation framework suitable for this kind of experimental simulation and outcome analysis.

SIMULATION RESULTS

The agents in MACSIMA log their internal status as well as their activities, negotiation steps and final outcomes in several separated and statistically evaluable data files. This raw data comprises information about the *evolution* of the agents' individual negotiation strategies, the course of negotiations together with their outcomes etc. This raw data can be easily transformed into diagrams that show the course of the evolution process of the agents' strategy parameters together with the emerging price fluctuations for the traded goods in the time elapsed.

Impacts of Evolutionary Adaptation

In our simulation runs conducted so far we have mainly concentrated on different instantiations of a five-tiersupply-network for computer manufacturing (see fig. 1). A first scenario has been defined in which genetic adaption was initially turned off and all agents were provided with the same static strategy parameter set $\langle A=0.5|DC=0.25|DJ=0.15|S=0.75|WM=0.2|R=1 >$ except for the processor producers whose acquisitiveness parameter *A* was set to 0.51 instead of 0.5.

The price fluctuations in the resulting simulation run – consisting of 300,000 simulation periods – are presented in the figure 6. Already the slight modification of the acquisitiveness leads to a strategic advantage for the processor agents and forces adjacent tiers to significant concessions.



Figure 6: Price Fluctuations with Learning Turned off

In a second simulation scenario we keep the settings of the foregoing scenario but exclusively provide the 10 processor producers with the ability to learn from previous negotiation outcomes. Their new learning capability empowers them to benefit much faster (see figure 7).



Figure 7: Learning Turned on only for Processor Agents

Emergence of Niche Strategies

As we can see in the figure 8, this effect is not achieved because all of the 10 processor agents follow the same strategy.



Figure 8: Emergence of niche Strategies

Instead of this, some agents of the processor tier benefit individually from following a niche strategy consisting in keeping the value of one's own acquisitiveness parameter slightly lower than the majority of the agents of the same type (see e.g. agents no. 1 and 6).

Agents of the same type but of lower acquisitiveness than their colleagues can benefit from this fact and increase their sales since their opponents expect no concession and thus accept quickly, if unexpected concessions are made.

Maximizing Profit and Turnover

We have examined whether there exists a parameterization by which - if applied by all the agents in a network - social welfare maximizing effects (i.e. an increase of the sum of the individual profits of all agents in a scenario) may be expected.

Therefore we have defined 50 simulation scenarios including two "baseline" scenarios each with a different parameterization of the learning process. For each scenario 4 simulation runs with 300,000 simulation periods each have been conducted. The means of some statistical variables from the 4 runs are shown in the figures 9 and 10.



Figure 9: Profit and Turnover in 50 Scenarios

In the first baseline setting learning was turned off for all agents and in the second the STDEA mechanism (Smith and Taylor 1998) was used by all agents. The evaluation results are shown in figure 9. An infelicitous parameter

choice results in a waste of welfare in such a way that overall turnover and sales may fall under the level of both baseline settings. Otherwise, an expert parameterization outperforms the first baseline by approximately 400 percent. The top parameterization we found (scenario 50 in figures 9 and 10) has the settings:

(pool_size = 3, population_size = 40, information_exchange = mixed, selection_method = roulette:wheel, recombination = n-point-crossover, mutation_rate = 0.5, Gaussian_width = 0.01, replacement_scheme = elitism).

Profit and turnover correlate with the number of successfully finished negotiations, i.e. transactions:



Figure 10: Negotiation Efficiency in 50 Scenarios

This is due to the fact that an expert parameterization of the learning process results in less negotiation break-offs since the agents adapt their negotiation behaviour better.

CONCLUSION & OUTLOOK

We have outlined some simulation results with a first focus on the emergence of niche strategies within a group of cooperating agents and a second focus on the effects of the application of different learning parameterizations on the overall profit of a networked supply economy instantiated by intelligent agents. The results demonstrate the suitability of the MACSIMA framework for modeling, simulating and analyzing complex economical scenarios. Our results show that, if one intends to use negotiating agents for coordinating a supply network one has to keep in mind that the parameterization of their learning mechanisms has to be fine-tuned for reaching an efficient and effective coordination outcome. Depending on the parameter setting the overall profit and turnover of a supply network coordinated by negotiating agents varies significantly. Further work will be directed towards a detailed analysis of the micro- and macro-effects (e.g. society loses welfare whereas certain individuals generate more profit) in dependence on varying learning parameterizations as well as information exchange and coalition formation settings.

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Ethological Concepts in Hierarchical Reinforcement Learning and Control of Intelligent Agents

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KEYWORDS

Agent, Simulation, Control, Reinforcement Learning, Ethology, Behavioral Approach, Artificial Life.

ABSTRACT

This paper integrates rigorous methods of reinforcement learning (RL) and control engineering with a behavioral (ethology) approach to the agent technology. The main outcome is a hybrid architecture for intelligent autonomous agents targeted to the Artificial Life like environments. The architecture adopts several biology concepts and shows that they can provide robust solutions to some areas. The resulting agents perform from primitive behaviors, simple goal directed behaviors, to complex planning. The agents are fully autonomous through environment feedback evaluating internal agent state and motivate the agent to perform behaviors that return the agent towards optimal conditions.

This principle is typical to animals. Learning and control is realized by multiple RL controllers working in a hierarchy of Semi Markov Decision Processes (SMDP). Used model free $Q(\lambda)$ learning works online, the agents gain experiences during interaction with the environment. The decomposition of the root SMDP into hierarchy is automated as opposed to the conventional methods that are manual. The agents assess utility of the behavior and provide rewards to RL controller as opposed to the conventional RL methods where the rewards situations map is defined by the designer upfront. Agent behavior is continuously optimized according to the distance from the agent's optimal conditions.

INTRODUCTION

Trend in artificial intelligence leans towards communities of robots - agents. These structures appears in nature in all types of complexity starting from genes, cells, multi-cell structures, through plants, animals, groups of animals up to their societies. Similarly to the Nature also in robotics it is obvious that one superintelligent robot (and therefore expensive) is with its abilities far behind a swarm of small, simple and less intelligent but also the less expensive robots. It is believed, that the power lies in quantity and simplicity. Also the range of possible types of tasks implemented on community of mutual cooperative robots is much

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) wider than in case of one super-robot. Therefore approaches from Artificial Life (ALife) are more often applied for control of community of robots. ALife approach (biological model) of implementation of intelligent behavior is inspired mostly by nature phenomena, instead of classical artificial intelligence (rational approach) which is more concerned about logic, rationality and just partially on algorithms inspired by nature. Another significant difference between AI and ALife approach is in the object of interest. Artificial intelligence is focused on complex thinking for example chess playing, text understanding, disease diagnostic etc. ALife if on the other hand focused on basic elements of natural behavior with strong stress on survival in environment. The most of existing ALife approaches are based on algorithms, which enables robots as artificially created creatures, to evolve and adapt (Kadlecek, Nahodil, 2001).

This article provides novel approach to a single agent architecture design. The primary motivation behind this research was to test the possibility of integrating rigorous methods of reinforcement learning and control engineering with behavioral (ethology) approach to agent technology. This work deals with a single agent architecture, rather then modeling multi-agent system. The main outcome of this research is an architecture called HARM designed for intelligent autonomous agents intended to behave in complex Artificial Life like environments. The term "Artificial Life like environments" prescribe environments where the agents are supposed to perform from primitive behaviors (e.g.: escaping from predators, eating, avoiding obstacles), simple goal directed behaviors (e.g.: finding water reservoirs), to complex planning (e.g.: assembling a shelter, getting through a maze with traps and riddles). The agent continually optimizes its behavior to increase its survival probability. Attainment of this goal depends mainly on how and how fast the agent can avoid danger, manage its own resources and gain resources from the environment. The agent shall be able to react to local disturbances and uncertainties, continuously improve its behavior and adapt to more persistent changes in the environment.

This research has been inspired by biology and by ethology and builds upon three fields:

Ethology/biology, control engineering and *reinforcement learning (RL).*

Ethology and biology gives the concept of animal behavior, homeostasis (self-regulation), motivation, and stimulation. Control engineering provides framework for modeling agent, its internal dynamics, and optimization through environmental feedback. RL [11] provides the agent with capabilities to learn and adapt its behavior in unsupervised manner on the basis of sparse, *delayed reward signals* provided when the agent reaches desired goals. *Hierarchical approach to RL* helps to combat complexity of the learning space that is typical for ALife environments.

DESIGN APPROACHES TO AGENT CONTROL ARCHITECTURE

Design approaches can generally be divided into three primary groups with this research following the hybrid paradigm:

- 1) Knowledge Based Architecture (Top-Down): Knowledge based architectures use knowledge to guide agent behavior. Much of the debate regarding the role of knowledge within an agent centers on how it is represented within the context of the control system. Steels [Steels, 1995] considers knowledge representations to involve "physical structures which have correlations with aspects of the environment representation (relationship with the external world) and thus a predictive power (ability to predict from actual knowledge) for the system". Agent modules are functional blocks like planning, learning or perception blocks and the behaviors (avoid obstacles, identify object, explore the environment) emerge from the interaction of the modules.
- 2) **Behavior Based Architecture (Bottom-Up):** Behavior based architectures build up the system of behavior producing modules instead of functional, as is the case in knowledge based architectures. Agent modules are behaviors such as avoid obstacles, identify object, and explore the environment. The functions of the system (planning, learning and others) emerge from the interaction of these modules and the environment. The most important phenomenon of behavior-based architectures is emergent behavior. Emergent behavior implies a holistic capability where the sum is considerably greater than its parts. Emergence is the appearance of novel properties in whole system and intelligence emerges from the interaction of the components of the system.
- 3) Hybrid Approach (Combined): Hybrid architectures integrate a knowledge-based component for planning and problem solving with behavioral components that produce robust performance in complex and dynamic domains. Strong evidence exists, that hybrid systems are found in biology, implying that they are compatible,

symbiotic, and potentially suitable for use in agent control. The focus of research in this area lies in defining an interface between deliberation and reactivity, which is poorly understood so far. Hybrid models include *hierarchical integration* and *coupled planning and reacting*.

BIOLOGICAL AND ETHOLOGICAL BASIS

This section introduces concepts I have reused from biology and ethology. Research of autonomous agents is being inspired by several disciplines. The study of animals and their behavior is among the main contributors. Animal behavior can be categorized into three major classes:

- **Reflexes** are rapid, automatic involuntary responses triggered by certain environmental stimuli. The reflexive response persists only as long as the duration of the stimulus. Further, the responsive intensity correlates with the stimulus's strength. Reflexes are used for simple activities or highly coordinated ones such as locomotion.
- **Taxes** are behavioral responses that orient the animal toward or away from a stimulus (attractive or aversive.) Taxes occur in response to visual, chemical, mechanical, and electromagnetic phenomena in a wide range of animals.
- **Fixed Action Patterns** (FAP) are time-extended response patterns triggered by a stimulus but persisting for longer than the stimulus itself. The intensity and duration of the response are not governed by the strength and duration of the stimulus, unlike a reflexive behavior.

Motivation: Behaviors are not governed only by environmental stimuli but also by the internal state of the animal (e.g. appetite). Motivation is a function of the interaction between internal and external factors (sources or stimuli). Internal conditions and external objects are both required for motivated behavior to appear. I.e. the incentive-value of an external object (e.g., a cookie) depends on internal conditions (e.g., need for calories).

Needs: Needs are internal physiological and psychological conditions that promote instigating drives. Needs can arise either from deprivation of internal body conditions essential to life (e.g., water or food) or to excessive stimulation. Physiological *need states*, *do produce corresponding drive states*, which motivate behavior and thereby assist animals and humans in maintaining homeostasis. An example of the *need* => *motivation* => *drive* => *behavior* => *inhibition feedback* loop of an animal is shown on the next scheme (Fig. 1).



Figure 1: Schema of the need => motivation => drive => behavior => inhibition feedback loop of an animal.

DESIGNED APPROACH

We have chosen the hybrid paradigm to agent architecture design. The system agent-environment works in self-regulation and self-optimization/learning loop. The agent receives feedback on its behavior from the environment. This environment feedback modifies agent's internal state that is together with agent's internal dynamics contained in the physiological system. Both the environment and agent respect physical laws and constraints. These physical laws and constraints are embedded in the physiological system also. The learning and control problem is represented as Semi Markov Decision Process (SMDP) or as multiple SMDPs. The agent learns optimal mapping of actions (or behaviors) to situations for each SMDP.

The framework of Reinforcement Learning (RL) is used for learning. Reinforcement Learning requires a priory mapping of rewards to situations. This mapping needs to be provided by the designer upfront. The common problem of this approach is that the designer brings in subjective experience and usually cannot define optimal mapping respecting both the agent internal model and properties of the environment. I have changed this concept in the sense that the agent evaluates rewards (action utilities) by itself. These rewards are derived from the transition in the agent's physiological space. If the action (or behavior) moves the agent towards its optimal conditions then the reward is positive and negative for reverse direction. Rewards are therefore aligned to real behavior utilities. This approach overcomes the problem of imbalanced and subjective mapping done by human designers. Main optimization criterion that is used during learning and control corresponds to agent's distance to the optimal conditions.

The agent decomposes the root SMDP to a hierarchy of multiple simpler SMDPs to simplify state space and speed up learning convergence. The decomposition leads to multiple SMDPs dedicated to specific behaviors from simple reactive ones to complex composite ones for planning. Motivation block then prioritizes those SMDPs that contain behaviors leading to correction of the agent's internal variables having the longest distance from optimal conditions. In the contrary to the conventional hierarchical reinforcement learning methods where the human designer is required to do the decomposition, I developed concept that allows the agent to make this decomposition automatically.

From a functional point of view, the agent holds properties depicted in Figure 2. Constraining properties of the environment are shown in the same figure.



Figure 2: Agent requirements and environment constraints

BEHAVIORAL ACCESS

Internal States

Agent properties and their dynamics (agent internal dynamics) is represented as a time invariant deterministic MIMO (Multiple Input-Multiple Output) system with the well known state-space model defined as:

$$\frac{dx}{dt} = f(x, u, t) \text{ and } y = g(x, u, t)$$
(1)

Where the state $x \in \mathbb{R}^n$ and the controls are $u \in \mathbb{R}^m$, $x \in X^A \subset \mathbb{R}^n$, $u \in \Omega \subset \mathbb{R}^m$ and $t_0 \le t \le t_f$.

 X^A represents *agent state variables*. An agent's internal state space fulfills the role of the physiological space of animals, and internal state variables correspond to animal's physiological variables. Physiological regulation processes in animals are realized through dynamics of the internal state system. From now on, the term physiological space can be used instead of the term internal state system.

balancing and behavior motivation grows nearly linearly. As the state approaches the lethal boundary, the motivation to return the animal back to balanced conditions increases. The "balancing" behavior is released when the animal's physiological state is close to the lethal boundary (*internal stimuli*) and the corresponding external releaser appears (*external stimuli*).

Motivation is a combination of:

- Internal stimulation that comes from the actual position in a physiological space
- External stimulation that comes from environment



Figure 3: Physiological space of an animal is used correspondingly in presented agent architecture.

Behavior Motivation

Animal's state can be represented as a point in its physiological space. An example of a two variable physiological space (e.g.: $x_1 \sim$ body temperature and $x_2 \sim$ blood pressure) is depicted in Figure 3 A. The state variables are most likely constrained and are determined by the animal physical properties and its environment. The space is bounded by the tolerance limits for these variables. A typical physiological space (Figure 3 A) contains three regions: (i) *limbo* – animal's conditions are almost optimal, (ii) *purgatory* – animal's conditions are critical, and (iii) *normal* area between these two where animal's (agent's) motivation is to perform

Internal stimulations increase from the origin towards boundaries of the physiological space. *Stimulation isoclines* line up the same level of internal stimulation. Figure 3 shows how an internal stimulation derived from multiple state variables and combined with external stimulations. The resulting motivation becomes the primary source for triggering behavior.

Stimulation isoclines line up the same level of motivation. Part 3 B) shows how internal stimulation depends on the agent's position in the physiological space. Part 3 C) shows the resulting motivation that is derived from internal and external stimulation.

Motivation is according to McFarland (McFarland, 1981) a function of internal and external stimulation.



Figure 4: Screenshot captured during experiments.

$$m = m\left(st_{int}, st_{ext}\right) \tag{2}$$

Where st_{int} is internal stimulation and st_{ext} is external stimulation. I represent stimulations as states of some selected internal and external state variables. Any motivation can result from multiple stimulations, thus the motivation function is a mapping from a set of internal and external variables to a real value:

$$m: X^{A} \cup X^{E} \to R \tag{3}$$

where X^{A} refers to agent internal variables, and X^{E} environment variables.

EXPERIMENTS AND OBTAINED RESULTS

Functionality of the designed agent architecture has been assessed in multiple focused experiments. In this paper, we discuss only the experiment demonstrating automatic creation of the hierarchies, learning and performing behaviors of different complexity in this hierarchy. In the experiment "The treasury problem", an agent needs to get to a treasure. The best action graphs are provided for *eat*, *drink*, *drop* and *get to treasure* behaviors. See Figure 4 with Artificial Life Simulator. Agent pushes boulders onto buttons to open the locked door and reach the treasure. In parallel, the agent satisfies its internal needs for food and water. Functionality of the designed agent architecture has been assessed in multiple focused experiments. In this paper, we discuss only the experiment demonstrating automatic and water. The graph (Figure 5) shows agent's learning convergence for "The treasury problem". The highest cumulative reward is obtained after the agent



creation of the hierarchies, learning and performing behaviors of different complexity in this hierarchy. In the experiment "The treasury problem", an agent needs to get to a treasure. The best action graphs are provided for *eat*, *drink*, *drop* and *get to treasure* behaviors. See Figure 4 with Artificial Life Simulator. Agent pushes boulders onto buttons to open the locked door and reach the treasure. In parallel, the agent satisfies its internal needs for food and water.

Note: The agent has no prior knowledge of the environment and no reward values are defined for the problem!

The agent must expose both planned behavior as well as primitive behaviors ensuring agent's survival. The

Figure 5. Graph of Mean Cumulative Reward

solves the "Treasury problem" and learns how to get to the treasure and satisfy its needs for water and food. The resulting graph (which shows agent's learning convergence) has staircase shape because of discrete points at which is received a new reinforcement type and the decision space is decomposed consequently.

The resulting hierarchy that the agent learns is depicted in another Figure 6. The agent has three internal variables: Food level, Water level and Obligation (used the express the need for fulfilling deliberative tasks), they produce three motivation functions: Food need, Water need and Fulfillment need.



resulting final hierarchy is created in about 8800 primitive actions and the agent is able to quickly find stones, carry them towards button, drop them onto the buttons, open the locked door and get to the treasure. At the same time, the agent can satisfy its needs for food

Figure 6: The decision space hierarchy automatically created for the Treasure problem

The root SMDP is automatically decomposed into a hierarchy of seven SMDPs as shown in the Figure 6.

Each SMDP is labeled as <Name> and a set of internal variables that are used for Q(lambda) learning in the concrete SMDP.

CONCLUSION

The main contributions of this research are seen in:

1. Showing how to integrate behavioral (bottom up) and deliberative (top down) approaches in a single agent.

2.Showing an approach how to bridge ethology/biology, agent technology, RL, and control engineering.

3. Showing that some concepts adopted from biology/ethology can be efficiently used as an alternative to classical approach.

4. Showing how to automatically decompose the root problem in a hierarchical RL as opposed to the conventional methods that need manual decomposition.

5. Showing how an agent can assess usability of its behavior and provide reward values to RL controller. This approach is different to the conventional RL methods where the rewards-situations mapping is defined by the designer upfront.

6. Presenting new method for evaluating optimality of agent behavior that is particularly useful in AL domain

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SIMULATING NORMATIVE BEHAVIOUR AND NORM FORMATION PROCESSES

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KEYWORDS

Norm innovation, Social simulation, Normative agents, Traffic scenario, Emergence, Immergence.

ABSTRACT

This paper describes the design of an agent model for simulating normative behaviour and norm formation processes. The model is based on a scientific theory of norm innovation, provided by the FP6 project EMIL (EMergence In the Loop). The main focus of the paper is the conversion of the theoretical framework towards a software implementation that can be applied for multiple simulation scenarios. A simple traffic scenario – where the traffic participants have to find rules to avoid collision incidents – serves as sample application.

INTRODUCTION

This paper focuses on the design and implementation of an agent-based simulation approach which describes the process of norm innovation, illustrated by a simple traffic scenario. It is part of the FP6 project EMIL (EMergence In the Loop: Simulating the two-way dynamics of norm innovation) as an example of simulating emergent properties in complex social systems, funded by the EU initiative "Simulating Emergent properties in Complex Systems" (no. 033841). The model design is based on a scientific theory of norm innovation, provided by EMIL (Andrighetto et al. 2007a). Using this theoretical framework, an agent-based norm innovation model is designed and implemented, which can be embedded in multiple simulation scenarios. A simple traffic scenario where the traffic participants have to find rules to avoid collision incidents - serves as a sample application. Dynamic model analysis as well as testing this norm innovation approach is supported by implementing the model using the agent-based traffic simulation tool TRASS (Lotzmann 2008).

THEORETICAL FRAMEWORK

The EMIL project especially focusses on understanding and analysing norm innovation processes in social systems, which can be seen here as a special case of complex systems, composed of many different interacting intelligent autonomous agents. In general, including norms in multiagent models seems to be a promising concept to understand human (and artificial) agent cooperation and co-ordination. Therefore, the design of agents with normative behaviour (i.e. normative agents) is of increasing interest in the multiagent systems research (Boella et al. 2007).

Because of the fact, that norms can be seen as a societal regulation of individual behaviour without sheer pressure, special attention in modelling and analysing norm innovation processes should be given not only to the inter-agent behaviour but also to the internal (mental) states and processes of the modelled agents (intra-agent) (Neumann 2008). Following this, the dynamics of norm innovation in EMIL can be described mainly by two processes:

- **emergence**: inter-agent process by means of which a norm not deliberately issued spreads through a society;
- **immergence**: intra-agent process by means of which a normative belief is formed into the agents' minds (Andrighetto et al. 2008).

From a more practical point of view, agent architectures, which are principally able to represent mental states and cognitive processes of agents, usually follow the (Belief-Desire-Intention) classical BDI approach (Bratman 1987). Even if an approach like the BOID (Belief-Obligation-Intension-Desire) architecture (Broersen et al. 2001) enhances this concept towards a more norm-like modelling by introducing an additional feature "obligation", the complexity of modelling and simulating norm innovation processes proposed in EMIL do not recommend the usage of such general and predefined architectures. This is because of the fact that all agent knowledge (beliefs, desires, intentions and especially obligations) are seen as predefined and "hardwired" agent properties. With these structures, it is impossible to answer questions regarding the origin of new norms or the communication of norms between agents (Campenni et al. 2008).

ARCHITECTURE OF A NORMATIVE AGENT

Concept

The prototype model of a norm innovation process presented here introduces normative agents, which are able to learn rules by observation and experience,

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supporting the identification of three main categories of norm innovation (Andrighetto et al., 2007b):

- Norm extension/adaption: Extending norms to new entities or social categories;
- Norm instantiation: Perceiving/Establishing a new norm;
- Norm integration: Determining norms by integrating conflicting norms.

For this purpose the essential communication between agents is based on a **message concept** (Figure 1) in which norm-related agent inputs (events and actions) are triggered by different message types (assertion, behaviour, valuation, sanction, ...).



Figure 1: Message structure

Messages and the corresponding events (included in the message component "Content") are divided into two groups:

- environmental messages/events (i.e. originating from the agent perception);
- norm invocation messages/events (i.e. notification or valuation received from other agents).

The processing of environmental messages (see section: Agent Behaviour) implements basically the (normoriented) behaviour of agents by selecting and executing actions coming from

- existing regular norms or
- · agent-related preliminary norms or
- the initial rule base (see section: Basic Structures).

The norm-invocation messages are in particular responsible for the **norm formation process**, which includes

- recognition of existing norms or agent-related preliminary norms by evaluating the valuation history of events;
- creation and adaption of preliminary norms by detecting regularities in event sequences and increasing/decreasing action probabilities;
- creation of regular norms by evaluating agentrelated preliminary norms.

Basic Structures

Agents.

The above mentioned processes require at least two kinds of agent-internal memories: Firstly, an **event board** memorizing a history of incoming environmental events including the conducted actions. And, secondly, a **normative frame** holding preliminary norms, derived from the event board as a result of the simulation. Finally, each agent needs an initial set of rules (**initial rule base**), which contains rules describing basic behavioural elements, and thus constituting the seeds for more complex rules emerging from the simulation process.



Figure 2: Event board

The event board is a chronologically sorted sequence whose elements contain the following data (Figure 2):

- the environmental message;
- the current (environmental) agent state (e.g. velocity and perception mode for a car driver in the traffic scenario);
- the associated action tree (see Figure 4) with the individual selection probability function.

At any point of time, the actual event board is characterized additionally by

• a classifier CLA (i.e. a value reflecting the similarity of different sequences independent from the chronological order or length), which will be calculated from a subsequence of the event board (starting from the recent event entry) and allows comparisons of subsequences in the norm formation process later on.

Each event board sequence describes a consecutive fragment of agent behaviour, thus introducing a higher level of complexity. It must be assumed that only within this complexity level, regularities and in particular norms are residing.

An entry of the normative frame, which can be given in advance by the modeller, or which arises from the detection of regularities in event board sequences, contains the following elements (Figure 3):

- the associated classifier of the event board sequence;
- the events from the corresponding event board sequence;
- a generated rule (a merged action tree);
- a valuation history, holding a statistical report of the valuations received on the respective rule.



Figure 3: Normative frame

Finally, each agent must be equipped with a set of initial rules, which allows him to act in the simulation environment. Rules in EMIL-S are represented as so-called **event-action trees**, which is a kind of decision tree that represents the dependencies between events and actions. For each event an arbitrary number of action groups are defined. Each action group represents a number of mutually exclusive actions. The edges of the tree are attached to selection probabilities for the respective action groups or actions (Figure 4).



Figure 4: Event Action Tree (For each action group $x \in [1..m]$ is $P_x \in [0..1]$; for actions $y \in [1..n]$ of action group x is $\sum y_x = 1$)

System Environment

On the system level an additional data structure is necessary, which contains regular norms, valid for the complete model. Again, this can be given in advance by the modeller or derived by the evaluation of preliminary norms from the agent's normative frames. Consequently, an entry of the normative frame (Figure 5) consists of the same elements as the normative frames, except of the validation history, which is used to decide, if a preliminary norm will become a norm or not.



Figure 5: Normative board

Agent Behaviour

Basically, the agent behaviour is determined by a process that is triggered by discrete events in the form of incoming messages. The contents of these messages can be events derived from the agent's perception, or advice from other agents dealing with valuations regarding events the agent is responsible for. Correspondingly, the process generates different outcomes: while in the former case mainly messages describing actions that the agent has to apply on his environment are produced, in the latter case actions that change the internal agent state are performed.

Thus, the first stage of the process is dedicated to the distinction of the incoming message type (by evaluating the message field "Modal") and the selection of the appropriate process. In this context, a perceptive event is called "environmental" (ENV), while the term for a valuation message is "norm invocation" (NI).

Beyond the obvious agent role of an "actor" (i. e. the addressee of the messages is the agent itself), the agent can also behave as an "observer", i.e. the agent monitors the message input from a subset of the agent population. The different inputs are treated as follows:

- for parts of the agent memory (namely the event board) several instances are necessary one for the actor role and one for each observed agent;
- the actions defined in the initial event-action-trees are attached with an role attribute, i.e. each role define distinct actions.

The two processes are now detailed in the following subsections with the help of UML activity diagrams.

Norm-oriented behaviour

Figure 6 shows the process for the case of an incoming environmental event.

At first, the event information is stored in a newly created event entry and inserted in the event board (EBx indicates an event board of agent "x") as latest entry. Based on this entry, the classifier (CLA) for the precedent time period is generated and stored as attribute of the event board.

This classifier is then used for lookup procedures in the normative data structures. In the first step, the (common) normative board (NB) is inspected.

If a norm with a similar classifier is found, then this entry will be copied into the normative frame (NFx) of the agent. In any case, the normative frame is searched for matching entries (which can be preliminary norms or norms copied from the normative frame) and finally one entry is selected (by an algorithm that reflects the agent's attitude against norms). This procedure is important to recognise typical and already known (complex) situations within the environment at an early stage to allow an adequate and timely reaction (e.g. to avoid undesired incidents). In case that no normative frame entry is found, the event-action-tree that belongs to the incoming event is fetched from the initial rule base (IRB).



Figure 6: Environmental event processing

In both cases, an action tree can be extracted: either from the normative frame entry, or from the eventaction-tree. This action tree is stored in the event board entry that was created at the beginning of the process (thus completing this entry) and afterwards evaluated for selecting and executing appropriate actions and therefore determining the agent's behaviour.

Norm formation

The process branch for an incoming norm invocation event is shown in Figure 7.

In this process, no entry for an event board is generated, but rather the actual event board (EBx) is searched for an event that is valuated by the incoming message. If no entry is found, then the valuation is invalid (for some reason, e.g. the valuated action is outdated and thus already removed from the event board). If an entry is found, it becomes the latest event of an event board subsequence for which a new classifier is generated.

This classifier is subsequently used for the same lookup procedures in the normative data structures as already described for the norm-oriented behaviour process: firstly, a possible adoption of a norm from the normative board (NB), and secondly, the search in the normative frame (NFx) for a matching entry. Again there are two possible results:

- No matching entry exists. In this case a new normative frame entry is generated by merging the event-action-trees from all elements of the event board sequence for which the classifier has been generated.
- There are one or more matching entries, from which the entry with the best conformity related to the classifier is chosen and the probabilities of the action tree stored in this entry are adopted in a reinforcement learning procedure.



Figure 7: Norm invocation event processing

This (either new or already existing) entry then undergoes a valuation history inspection (after the current event was added to the valuation history) with the objective to decide whether the preliminary norm can be transformed into a regular norm. This decision algorithm considers

- from how many different agents valuations are stored in the valuation history, and
- the change rates of the probabilities attached to the action tree during the recent time period.

If the agent decides to transform the preliminary norm into a norm, the content of the normative frame entry will be copied to the normative board (NB). Thus a new norm has emerged.

IMPLEMENTATION REMARKS

In the final section a few remarks on design aspects as well as hints on the implementation progress of the simulation software, and a simple simulation scenario are given.

System Architecture

The norm formation process described in the previous section is the basis for the agent implementation in the EMIL-S simulator.



Figure 8: Component diagram of the entire simulation suite

EMIL-S is not realized as a stand-alone software, but rather as a supplemental component of a larger system (Figure 8), consisting of a general purpose simulation tools such as REPAST (North et al., 2006), MASS (Ivanyi et al., 2007b) or TRASS (Lotzmann and Möhring 2008; Lotzmann 2009) and an experimentation environment such as MEME (Ivanyi et al., 2007a), a tool for automated simulation execution with build-in parameter sweep functionality.

EMIL-S Agent Designer

From a modeller's point of view an EMIL-S model can be described completely by a set of event-action trees, which serve as an initial rule base for the initialized agents and provide them with norm formation abilities.

To support the usage of this generic "modelling language", the simulation suite provides a user interface (Figure 9), which facilitates the input of event-action trees (and allows the observation and analysis of simulation runs later on).



Figure 9: User interface: Model designer, displaying an event-action tree from the initial rule base

At present, the concept of describing norm formation models by event-action trees is tested by transforming different model scenario into this language concept. Examples:

- Traffic scenario (see below, completed)
- Wikipedia scenario (Troitzsch, 2008; completed)
- Microfinance scenario (Anjos, 2008; in progress)
- Scenario on conformity in multiple contexts (Andrighetto et al., 2008; in progress)

Connecting EMIL-S with Simulation Tools

The link between the EMIL-S and the simulation tool is defined by an interface which allows the integration of an EMIL-S strategy layer into agents implemented within the simulation tool. Given that an adequate agent architecture is present on the simulation tool level this can be seen as an approach for realizing embodied agents. Figure 10 shows an example of such an architecture.



Figure 10: Integration of EMIL-S in TRASS

EMIL-S acts as the strategy layer in cooperation with the "robotics" and the "physical" layers of the TRASS framework.

An example for the combination of EMIL-S and TRASS is shown in the following section: a simulation scenario, dedicated to explore the formation of traffic norms as a result of interactions between car drivers and pedestrians.

Traffic Scenario

The field of microscopic traffic simulation is dominated by agent-based approaches which are focusing on precise mathematical modelling of physical parameters. In many cases, the interaction between traffic participants is restricted to measuring and keeping distance with the aim to avoid collisions (as e.g. implemented in classical car-following models). Psychological aspects of traffic participants as well as social relations between them are much less treated in current approaches, although these are crucial factors for the dynamics of any real traffic system in which usually various kinds of traffic participants (drivers, cyclists, pedestrians, ...) appear. In particular, social capabilities are the key for integrating differing perspectives (of distinct kinds of traffic participants) on a joint event.

Normative behaviour and learning introduces social capabilities for agents in traffic simulations. The following model is a step toward this more comprehensive view on traffic systems.

The traffic scenario (Lotzmann et al., 2008) consists of a simple topography, which is composed of a straight oneway road and two meadows to the left and right of the road. A small segment of the road has a special mark (much like a crosswalk). Situated within both meadows, a number (which is constant during a simulation run) of pedestrian agents move around. From time to time each pedestrian gets an impulse to reach within a given period of time a target point on the opposite meadow. For this activity, the agent can choose between the direct way to the target or a detour via the crosswalk. The road is populated by car agents who are aimed at reaching the end of the road at a given point of time.

For both types of agents, the deviation from the permitted duration leads to a valuation of the recent agent activity: a penalty when more time was required and accordingly a gratification when the target was reached earlier.

Due to the interaction between agents, occasional collisions are likely to happen. Such an event, when occurring between a car and pedestrian, is classified as undesirable. Observations of a collision provoke other agents to issue sanctions against the blameable agents. The extent of the sanction is determined by various factors reflecting the environmental situation (e.g. the road section where the collision occurred) and the normative beliefs of the valuating agent (e.g. a collision on a crosswalk might result in a harder sanction than on the rest of the road). Sanctions lead to a temporary stop of motion for the involved agents. Hence, to avoid

sanctions is a competing goal to the aforementioned aims (reaching the target point or end of the road, respectively, in due time).

To map this informal concept into the EMIL frame, a classification of the expected information transfer to message types is necessary in a first step. Every agent is able to perceive its environment and to conduct actions in order to adjust the (own) parameters of motion or respectively. These (agent perception. internal) processes can be mapped to message modals "assertion" and "behaviour". In addition, agents can send and accordingly receive messages to/from other agents. The contents of the messages are different kinds of notifications (like positive or negative valuations and sanctions, e.g. "admonish" or "honk the horn"...). While these message exchanges are either intra-agent matters or speech acts between exactly two agents, another agent property is important for a norm formation process. This is the ability to listen to the communication of other agents in order to gain information about the experience of those agents, and to learn from this information.

With regard to this message classification, rules for the specification of agent behaviour have to be defined in a second step. The structure of a rule follows an event-action scheme where events trigger actions from an action set with certain probabilities. In this model, all events are coupled with received messages and most actions are expressed by message sending activities. Furthermore, additional actions for learning have to be defined.

All rules are constructed with the help of event-action trees. Figure 11 shows a sample event-action tree for a car driver agent.



Figure 11: Event-action tree with environmental actions

While the structure of the scenario-specific (initial) event-action trees is static, the selection probabilities may change during the simulation in a learning process. Furthermore, more complex rules can emerge by linking several event-action trees. With these behavioural rules, norms emerge as soon as the majority of the population starts to use the same rules with similar probability distributions.

Finally, Figure 12 shows a screenshot of a simulation run after a longer learning period. There are 20 pedestrian agents observable, heading towards the target. The majority of the pedestrians use the crosswalk to cross the road, while a minority chose the direct way. The reason for using the crosswalk in spite of a potentially longer route is due to the observation that car
drivers usually stop in front of crossroads while they are ignoring pedestrians waiting at an ordinary road segment. Even this behaviour of the car drivers is result of a learning process due to a higher number of collision incidents in crosswalk-sections.



Figure 12: Simulation run screenshot

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AFFECTIVE AGENTS PERCEIVING EACH OTHER'S ACTIONS

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ABSTRACT

In this paper, an extension of a formalized model of affective decision making is presented, based on the informally described I-PEFiC model. This extension manages that the actions agents undertake have an effect on other agents. The agents change their perceptions and beliefs about other agents if actions are taken. Further, the anger level of the agents is simulated. Simulation experiments show that the actions of agents can change the beliefs and the perceptions of another agent so much that the other agent changes its mind and chooses to perform another action than it was currently doing.

INTRODUCTION

From the last decade, a lot of research has been dedicated to developing Intelligent Virtual Agents (IVAs) with more realistic graphical representations. However, these agents often do not show very realistic human-like emotional behavior. For example, many IVAs can show emotions by the means of facial expressions or the tone in their voice, but most of them still struggle to show the right emotions at the right moment (e.g., emotion regulation (Marsella and Gratch 2003) and moods (Beck 1987)). Let alone actually understanding and reacting empathically to the emotional state of other agents, or human users. Previous research has shown that closely mimicking humans is important for an agent to increase human involvement in a virtual environment (e.g., Van Vugt et al. 2006).

From Frijda's point of view, emotions are goal driven (Frijda 1986). The emotional system examines the surroundings for related stimuli that are either beneficial or harmful for the concerns, motives, and goals of the individual (Frijda 1986, p. 494, p. 463). According to broaden-and-build theory, positive emotions are vehicles for individual growth and social connections: by building people's personal and social resources, positive emotions transform people for the better, giving them better lives in the future (Fredrickson 2001, p. 224). Previous research also showed that human beings Ghazanfar Farooq Siddiqui VU University, Amsterdam Center for Advanced Media Research Amsterdam De Boelelaan 1083, 1081HV, The Netherlands ghazanfa@few.vu.nl www.few.vu.nl/~ghazanfa

usually make unconscious rather than conscious decisions (Bargh and Chartrand 1999).

We created agents for imitating human behavior, who can recognize each other as a personal friend as well as means to an end. The Interactive model of Perceiving and Experiencing Fictional Characters (I-PEFiC), which is based on the theory of Frijda (Frijda 1986), was taken as a foundation with regard to recognizing each other as a personal friend (Van Vugt 2008). Within this model an agent A can compute the trade-off between how involved it is with another agent (e. g., Agent B is good) and what keeps the agent at a distance (e. g., Agent B is bad) (Bosse et al. 2008). This involvement-distance trade-off is the outcome of assessing the features of an agent on several dimensions. Use intentions are calculated additionally that prompt the agent to carry out actions towards another agent.

These actions are based on goals, which play a role in the judgment formation of the agent about the other agent, but also more affective influences are taken into account. The previous decision making model (Hoorn et al. 2008) only describes the affective decision making process itself. Simulation experiments with this model showed that in situations where this can be considered human-like, agents make affective decisions rather than decisions that would be the best rational decision (i. e., the decision option with the highest expected utility). However, it did not explain the effects of the performed actions on the agents' perceptions, beliefs and levels of anger. Neither did it explain how these changed beliefs and perceptions influenced the following decision making processes.

In this paper we improved the affective decision making model (Hoorn et al. 2008), so that the agents update their beliefs and perceptions of the ethics and affordances of other agents when actions are being performed. Further, the effects of these actions on the emotions of the agents are simulated. These changes on their turn influence the decision making process in the agents. This enables the agents to change their mind and decide to change the action they want to perform. The simulation experiments described in this paper will show what kind of effects the actions have on the agents' beliefs, perceptions, and emotions and how this affects their decision making.

MODELLING APPROACH

Modelling the various aspects involved in affective decision making in an integrated manner poses some challenges. On the one hand, qualitative aspects have to be addressed, such as performing an action. On the other hand, quantitative aspects have to be addressed, such as levels of anger. The modelling approach based on the modelling language LEADSTO (Bosse et al. 2007) fulfils these needs. It integrates qualitative, logical aspects such as used in approaches based on temporal logic (e. g., Barringer et al. 1996) with quantitative, numerical aspects such as used in Dynamical Systems Theory (e. g., (Ashby 1960), (Port and Gelder 1995)).

In LEADSTO, direct temporal dependencies between state properties in two successive states are modelled by executable dynamic properties defined as follows. Let **a** and **b** be state properties of the form "conjunction of literals" (where a literal is an atom or the negation of an atom), and **e**, **f**, **g**, **h** non-negative real numbers. Then in the leads to language $\mathbf{a} \rightarrow_{\mathbf{e}, \mathbf{f}, \mathbf{g}, \mathbf{h}} \mathbf{b}$, means:

If state property a holds for a certain time interval with duration g, then after some delay (between eand f) state property b will hold for a certain time interval of length h.

Here, atomic state properties can have a qualitative, logical format, such as an expression desire(d), expressing that desire d occurs, or a quantitative, numerical format such as has_value(x, v) expressing that variable x has value v.

IMPLEMENTATION

I-PEFiC is a model (Figure 1) that is empirically well validated (Van Vugt et al. 2006, Van Vugt et al. 2007, Van Vugt 2008). The I-PEFiC model has three phases: encoding, comparison, and response (Van Vugt et al. 2007).

During encoding, the user appraises an agent's features for their level of ethics (good or bad), aesthetics (beautiful or ugly), and epistemics (realistic or unrealistic). During the encoding, moreover, the user evaluates in how far the agent system has affordances (aids or obstacles), which make the agent useful as a computer tool or not.

In the comparison phase, the features are judged for similarity (similar or dissimilar) (e.g., "I am not like the agent"), relevance of features to user goals (relevant or irrelevant) and valence to goals (positive or negative outcome expectancies). The measures in the encode phase - moderated by the factors in the comparison phase - determine the responses, that is, the levels of involvement with and distance towards the embodied agent. Moreover, the intention to use the agent as a tool indicates actual use and together with involvement and distance, this determines the overall satisfaction of the user with the agent; in our case of Agent A with Agent B. The I-PEFiC model has been formalized in (Bosse et al. 2008).



Figure 1: Graphical Representation of I-PEFiC

The model presented in this paper is an extension of a model of affective decision making (Hoorn et al. 2008) based on a formalization of the I-PEFiC model (Bosse et al. 2008) in the LEADSTO environment (Bosse et al. 2007). In this decision making model, decisions are made based on rational as well as affective processing. In the model an agent has desired and undesired goalstates. The agent perceives affordances of the other agents by means of beliefs that the agents facilitate or inhibit reaching certain goal-states. These perceived affordances of other agents are compared to the goalstates it wants to achieve or avoid. While doing this, it can reason about the outcome expectancies of using the other agent for a certain action (e. g., comforting, fighting, or criticizing). In humans, such outcome expectancies lead to certain quick and mostly subconsciously generated action tendencies. In our agents, as in humans, action tendencies influence the experienced involvement and distance towards the other agent. The involvement and distance towards another agent are combined with the use intentions of that agent and the expected utilities of the possible actions to calculate the expected levels of satisfaction of these actions. These expected levels of satisfaction are compared to reach a final decision that is based on rationality as well as affective influences.

We created a library of actions the agents can perform. In this action library, the type of each action is specified. Actions can be specified as

- (1) Positive approach
- (2) Negative approach
- (3) Change
- (4) Avoid

In this paper, the action library consists of one action for each type. Comfort is an action of the type positive approach, fight is an action of the type negative approach, criticize is an action of the type change, and avoid obviously is an action of the type avoid. If an agent tries to perform an action of type 1, 2, or 3 towards another agent, while the other agent is avoiding the agent, it will not succeed in performing this action. If an agent performs an action towards another agent, this affects the agent that is the object of the action, as well as the agent that is performing the action itself. The formulas and values not described in this paper can be found in http://www.few.vu.nl/~mpontier/ECMS-2009-Appendices.pdf.

Adjusting the perceived ethics

If an agent performs an action towards another agent, the agent that is the object of the action can change its perception of the goodness and badness of the agent performing the action. For example, if an agent fights another agent, the agent that is the object of this action will probably decrease its perception of the goodness of the fighting agent, and increase its perception of the badness of the fighting agent. To establish this change in perception, the bias (in the range [0, 2]) changes according to the actions that are being performed. A bias > 1 means overestimation, and a bias < 1 means underestimation. To calculate the effect of an action on the bias for perceiving the goodness of the agent performing the action, we have developed the following formula:

new_bias(good) = p_{good} * old_bias(good) + (1-p_{good}) * v_(agent, action, good)

In this formula, new_bias(good) is the new value of the bias, old_bias(good) is the old value of the bias, and the persistency factor p_{aood} is the proportion of the old bias that is taken into account to determine the new bias for perceiving goodness of the agent that is performing the action. In this paper, for clarity in the simulation experiments this persistency factor is set to 0.85 for all agents, but this could just as easy be personalized per agent. The new contribution to the bias is $V_{(agent, action, action)}$ good), a value that an agent attaches to the goodness of being the object of the performed action. In practice this means that if a certain action is performed towards an agent, the bias of good will move towards the value the agent attaches to being the object of that action. In this paper, all the agents attach the same, arbitrarily chosen values to being the object of actions, but also this could easily be personalized per agent. As the biases are in the range [0, 2], these values are also in the range [0, 2]. The values can be found in Table 1.

Table 1: The Values of Goodness the Agents Attach to Being the Object of an Action

1	1
Action	Value
Comfort	1.5
Fight	0.5
Criticize	1.25
Avoid	0.75

The actions for calculating the effect of an action on the bias for perceiving badness are calculated in a similar way as the effect on the bias for perceiving goodness. The only difference is that the values used in this formula are the values the agents attach to the badness of being the object to the performed action. These values can be found in Table 2.

new_bias(bad) =

p_{bad} * old_bias(bad) + (1- p_{bad}) * v_{agent, action, bad}

Table 2: The Values of Badness the Agents Attach toBeing the Object of an Action

Action	Value
Comfort	0.5
Fight	1.5
Criticize	1.25
Avoid	1.25

Adjusting the perceived affordances

If an agent performs an action towards another agent, the agent that is the object of the action can also change its beliefs about the affordances of the agent performing the action. Beliefs have a value in the domain [-1, 1]. A belief of 1 represents a strong belief that the statement the belief is about is true, and a belief of -1 represents a strong belief that it is not true. For example, if an agent fights another agent, the belief that avoiding the other agent helps to reduce your anger might increase. To calculate the effect of an action on beliefs about the agent performing the action, we have developed the following formulas:

if beliefchange \geq 0: new_belief = old_belief + belief_adaptation * beliefchange * ((1 - old_belief) / 2)

if beliefchange < 0: new_belief = old_belief + belief_adaptation * beliefchange * ((1 + old_belief) / 2)

In these formulas, new_belief is the new value of the belief, old_belief is the old value of the belief, and belief_adaptation is a variable, set at 0.1, that determines the speed with which the beliefs are changed when being the object of an action. The beliefchange is a variable in the range [-1, 1] that determines the change of a belief about the performing agent when an agent is performing an action, or is the object of an action performed by another agent. Multiplying with ((1 - old_belief) / 2) when beliefchange is positive, and with ((1 + old_belief) / 2) when beliefchange is negative manages that the values of the beliefs change less if they approach their boundaries, and prevents them from going out of the domain [-1, 1]. In this paper, the values for beliefchange are the same for all agents,

but this could easily be personalized per agent. All beliefchange values can be found in Table 3.

In this table, in the columns the actions that are the cause of the belief change are shown. In the rows the affected beliefs are shown. These beliefs are about an action facilitating a certain goal. For example, if an agent A fights another agent B, agent A will change its belief that comforting agent B will help to reduce his own anger with a beliefchange value of -0.75, as can be seen in Table 3.

Table 3: The beliefchange	Values when Actions Are
Perfor	med

Affected Belief		Actions causing the belief change			
Action	Goal	Comfort	Criticize	Fight	Avoid
Comfort	Self	0.2	-0.2	-0.75	-0.6
Criticize	Self	-0.5	0.9	-0.5	0.6
Fight	Self	-0.9	0.3	0.75	0.4
Avoid	Self	-0.25	0.8	0.9	0.7
Comfort	Others	0.4	0.2	-0.5	-0.3
Criticize	Others	-0.25	-0.25	0.25	-0.4
Fight	Others	-0.8	-0.8	0.25	-0.7
Avoid	Others	-0.35	-0.6	0.75	0.8

Adjusting the emotions of the agents

The actions that an agent performs, and the actions that are performed to an agent, affect the emotions of that agent. The emotion simulated in this paper is the level of anger, but also other or even multiple emotions could be simulated in a similar manner. To calculate the effect of actions performed on the anger level, we have developed the following formula:

new_anger = $p_{anger} / n * old_anger + (1 - p_{anger} / n) * \Sigma(changed_anger) / n$

In this formula, new_anger is the new anger level, and old_anger is the old anger level. The persistency factor p_{anger} is the proportion of the old anger level that is taken into account to determine the new anger level. In this paper, for clarity in the simulation experiments, this persistency factor is set to 0.95 for all agents, but this could easily be personalized per agent. The number of actions that is taken into account for calculating the new anger level is represented by n. The persistency factor is divided by n, so that there will be less persistency in the anger level if multiple actions are taken into account.

The new contribution to the anger level is the mean of all the changed_anger variables that are attached to the actions taken into account. This changed_anger is a variable that indicates which value the anger level approaches given a certain action. In practice this means that if a certain action is performed towards an agent, the anger level will move towards the value of the changed_anger attached to that action. For example, if an agent fights another agent, this will make its anger level approach 0.7, because if the anger level is very high, fighting another agent might help to release this anger, although it will never help to decrease it to a low anger level. On the other hand, if an agent has a low anger level, fighting another agent will probably increase the level of anger.

In this paper, all the agents attach the same changed_anger values to actions, but it would be just as easy to let each agent have its own personal values. As the anger levels are in the range [0, 1], the changed_anger values are also in the range [0, 1]. The values used for this paper can be found in Table 4.

Fable 4: The changed_	_anger Values the Agents
Attach to Sp	ecific Actions

Action	Value if subject	Value if object
Comfort	0.2	0.2
Fight	0.7	0.9
Criticize	0.2	0.6
Avoid	0.3	0.7

SIMULATION EXPERIMENTS

The simulation model introduced in the previous section was used to perform a number of experiments under different parameter settings. In the experiments, the three agents Harry, Barry, and Gary followed a (fictitious) anger management therapy. An infinite number of actions could be inserted in the system, but for clarity, nonetheless, for each action type we inserted only one instance of an action. The action to comfort another agent is a type of positive approach whereas the action for negative approach was to fight another agent. Criticizing another agent was the action associated with change, and the action for avoiding the agent was to simply move away from another agent. In the simulation experiments, a calculation step takes one timepoint and an action takes five timepoints. After these five timepoints the action taken can be reconsidered and changed. The results of the experiment are described below. Notice that in each graph in this paper, the scale on the y-axis can differ.

We expected that the system can generate simulations in which actions lead to changes in perception in such a way, that agents change their mind and perform another action than they would have done before their perception was changed.

Experiment 1: Baseline

To start, an initial experiment was performed that served as a control condition for the rest of the experiments. In this experiment, the designed features for beautiful and ugly (aesthetics), good and bad (ethics), and realistic and unrealistic (epistemics) are all set to 0.5 (see Figure 1). All biases for perceiving these features are set to the neutral value of 1. The agents have no beliefs about other agents (all beliefs are set to 0), and the only ambition they have is to reduce their own anger with an ambition level of 0.5.



Figure 2: Simulation Results of Experiment 1

In Figure 2, along the X-axis the timepoints are shown, and along the Y-axis several statements are shown. A dark blue bar means the statement holds at that timepoint, and a light blue bar means the statement is false at that timepoint. As can be seen in Figure 2, these settings result in Barry and Harry avoiding Gary, and Harry avoiding Barry after timepoint 11.



Figure 3: Harry's Involvement, Distance, Perceived Goodness and Perceived Badness of Gary

As can be seen in Figure 3, the agents who are being avoided increase their distance from 0.49 to 0.82, and

decrease their involvement from 0.44 to 0.28 towards the avoiding agent. This happens because the perceived goodness of these agents decreases from 0.5 to 0.38 and badness increases from 0.5 to 0.62. Being avoided also causes changes in beliefs.



Figure 4: The Beliefs of Barry about Harry during Experiment 1.

As can be seen in Figure 4, the agents who are being avoided start to think that avoiding, criticizing, or fighting the avoiding agent will help them to reduce their own anger, and that comforting the avoiding agent will inhibit their goal of reducing their own anger. As initially the agents have no beliefs about each other, the agents have no intentions to use each other at the start of the simulation.



Experiment 1.

Because the agents that are being avoided start to have beliefs about the avoiding agents, their intentions to use that agent also increase from 0 to 0.46, as can be seen in Figure 5.

Being avoided also changes the anger level. As can be seen in Figure 6, the anger level of Barry decreases from 0.60 to 0.50, and the anger level of Harry decreases only from 0.60 to 0.57 (notice the differences in scale on the y-axis). Harry's anger level decreases less because he is avoided by both Barry and Gary. Gary's anger level reduces to 0.30, which is even more than that of Barry, because he is not being avoided by any agent. This shows that being avoided by multiple agents has a greater impact than being avoided by only one agent.



Figure 6: Anger Levels of the Agents in Experiment 1

Experiment 2: Harry beliefs he should not avoid Barry

We performed an experiment in which Harry has a strong belief (value = 1) that avoiding Barry will inhibit his goal of reducing his own anger. Harry also has a stronger ambition to reduce his own anger, with a value of 1 instead of 0.5. The remaining variables have the same values as in the baseline condition.



Figure 7. Simulation Results of Experiment 2.

Due to this, instead of avoiding Barry, Harry now tries to comfort Barry at time-point 11, as can be seen in Figure 7. However, he does not succeed in comforting Barry, as Barry is avoiding Harry, just like in the baseline experiment. This causes Harry to stop avoiding Barry at time point 16 and increases his anger level to from 0.53 to 0.70, as can be seen in Figure 8.

Not being comforted anymore also slightly increases Barry's anger level from 0.25 to 0.27 in the five following time steps. In the mean time, Barry has observed that Harry tried to comfort him, which decreases his anger level from 0.60 to 0.25. It also changes his perceptions of the ethics of Harry. As can be seen in Figure 9, Barry starts to see Harry as a good guy, with a perceived goodness of 0.64 and a perceived badness of 0.36.



Figure 8: Anger Levels of the Agents in Experiment 2





Figure 9: Barry's Perception of the Ethics of Harry during Experiment 2



Figure 10: Barry's Involvement and Distance towards Harry during Experiment 2

This also slightly increases Barry's belief that comforting Harry will help him to reduce his anger, while his beliefs that avoiding, criticizing or fighting Barry will help him to reduce his own anger are slightly reduced.

These changes in beliefs and perceptions cause the involvement of Barry towards Harry to increase from 0.44 to 0.56 and the distance from Barry to Harry to decrease from 0.50 to 0.34, as can be seen in Figure 10. This causes him to start comforting Harry instead of avoiding him at timepoint 21.



Figure 11: Harry's Perception of the Ethics of Barry during Experiment 2

However, in the mean time, being avoided by Barry has changed Harry's opinion about him. The perception of his goodness has decreased from 0.50 to 0.39, and the perception of his badness has increased from 0.50 to 0.61, as can be seen in Figure 11.



Experiment 2

As can be seen in Figure 12, also Harry's beliefs that fighting, criticizing, and especially avoiding Barry will help to reduce his own anger increase, whereas his belief that comforting Barry will help to reduce his own anger decreases. In the mean time, being avoided by Gary has decreased Harry's involvement towards Gary, increased his distance towards Gary, and has increased his beliefs that criticizing, fighting, or avoiding Harry will help him to reduce his own anger in a similar way as in experiment 1.





20 30 40 50 60 70 80 90 100

0.35

As can be seen in Figure 13, this increases Harry's expected satisfaction of performing an action towards Gary, namely avoiding him, and this expected satisfaction exceeds the expected satisfaction of performing an action towards Barry. This causes Harry to change his mind and start avoiding Gary at timepoint 26. In the mean time, after Barry started to comfort Harry at timepoint 21, Harry's anger level decreases from 0.70 to 0.40, and Barry's anger level from 0.28 to 0.20.

Also the distance from Harry to Barry decreases from 0.66 to 0.09 and his involvement increases from 0.37 to 0.67, as can be seen in Figure 14. This happens due to an increase in Barry's perception of Harry's goodness from 0.39 to 0.75 and a decrease in perceived badness from 0.61 to 0.25, and because his increasing belief that comforting Harry will help him to reduce his own anger, and fighting, criticizing or avoiding Harry will inhibit his goal to reduce his own anger.



Figure 14: Harry's Involvement and Distance towards Barry during Experiment 2

DISCUSSION

In this paper, we presented an extension of a formalized model of affective decision making (Hoorn et al. 2008), based on the informally described I-PEFiC model (Van Vugt et al. 2006, Van Vugt et al. 2007, Van Vugt 2008). This extension manages that the actions the agents undertake have an effect on the agents. The agents change their perceptions and beliefs about other agents if actions are taken. Further, the anger level of the agents is being simulated. Simulation experiments have been performed to show how the actions affect the agents. Experiment 1 showed that if multiple agents perform an action towards another agent, this has a bigger effect on its anger level than if only one agent would perform that action. Experiment 2 showed that if an agent performs an action towards another agent, this can change the beliefs and the perceptions of the other agents so much that the other agent changes its mind and chooses to perform another action than it was currently doing, leading to a completely different situation than in experiment 1, confirming our expecations as mentioned in section 4. These results are as would have been expected from the theory (Hoorn et al. 2007, Van Vugt et al. 2006, Van Vugt 2008).

In this paper, the simulation experiments are performed in the domain of anger management therapy. The only simulated emotion is anger, and for each type of action there is only one possible action to perform. However, this model could be used for any type of domain, with other, or multiple emotions simulated at the same time. Also as many actions as desired could be added to the action library. This way, the model could be used to perform simulations involving decision-making, emotions, and changing perceptions for any domain.

Of course, a lot of additions could still be made to our model. For instance, the persistency factors for changing the beliefs and perceptions of other agents could be made dependent on the period of time the agents know each other (or on the number of interactions). Existing models of decision-making usually assume this process to be rational, which would exclude the possibility of emotions playing a role other than disturbing the process (Gutnik et al. 2006). However, humans often make irrational decisions. A good example for this is the Ultimatum game (Thaler 1988), for which behavioral research showed that low offers (20% of total amount) have a 50% chance of being rejected. Participants reported that they found low offers unfair, and therefore out of anger they selected the irrational option (Gutnik et al. 2006).

Models of decision making usually have a hedonic bias, and generally try to find the action with the highest expected utility. Some decision theoretic models, such as (Gmytrasiewycz and Lisetti 2001), take emotions into account, but in those models, emotions merely confirm good rational decisions – emotional states as modes of decision making. However, these models cannot explain irrational behavior, where actions with a (relatively) low expected utility are chosen. Our balancing model takes the expected utility as well as involvement-distance trade-offs into account. This way, situations in which emotions overwhelm rationality can be explained and simulated.

There have been a number of approaches to model decision-making based on emotions in autonomous agents. However, none of these studies uses a detailed model of perception of others to explain how these affective influences in the decision making process are generated. Usually, these models somehow assume that emotions are there. For instance, (Velasquez 1998) presents a model of emotion-based decision-making, which is an extension of a previous model (Velasquez 1997). The model that is presented in this paper assumes a perceptual system, but how this perceptual system actually works is not considered in the paper.

Ahn & Picard (Ahn & Picard 2005) present a computational framework of affective-cognitive learning and decision making for affective agents. This model integrates affect and cognition, where 'internal rewards from cognition and emotion' and 'external rewards from the external world' serve as motivations for learning and decision making. In this model emotions are generated based on these rewards, but perceiving others in the world is left out of consideration.

In future research, we plan to combine the model with an existing computational model for emotion regulation (Bosse et al. 2007). Whereas the current model focuses on the elicitation of emotion, that model addresses the regulation of emotion. Further, we intend to explore where these models and the EMA model (Gratch and Marsella 2004) complement each other, and use this to further refine the models.

Finally, in a later stage of the project, we will confront our formalization with empirical data of human affective trade-off processes. As soon as the model is validated and adapted, we will start exploring the possibilities to build a robot that can interact with real humans. We hope to develop a robot that can communicate affectively with humans in a more natural way, that is, with a mind of its own, in pursuit of its own goals, and acting emotionally intelligent.

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MULTIAGENT DECISION MAKING FOR SME SUPPLY CHAIN SIMULATION

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KEYWORDS

Small and Medium Enterprises (SMEs), Supply chain, multiagent, modelling, reactive monitoring.

ABSTRACT

To tackle the complexity and heterogeneity of the networks that integrate Mechatronic SMEs, this paper describes a modelling and simulation solution based on multiagent system and ArchMDE (Architecture Model Drive Engineering) methodology for supply chain agentification. This research work outlines two main results: conceptualisation and modelling. The first one deals with the identification and concepts definition of the different entities moving and acting into the multiagent and supply chain systems. The second one discusses the agent approach providing a framework naturally oriented to model supply chain concepts and their dynamic behavior.

INTRODUCTION

The Supply chain concept has become a major stake in today's industrial context. In order to meet the dynamic global market and its requirements, Small and Medium Enterprises (SMEs) must integrate supply chain practices in their own complex network [Villarreal Lizarraga *et al.*, 2005; Julien, 1997].

In the French region of Savoie, the industrial environment is mostly composed of particular SMEs specialized in mechatronics. Very often, these companies collaborate in a cluster to achieve a task in the global supply chain. Indeed, according to some investigations and studies on the environment, three major features of the supply chain which integrates SMEs cluster and especially mechatronic ones [Tounsi et al., 2008] arose. Firstly, supply chain in this context is a complex system. This complexity is due to the high number of autonomous actors and SME networks which collaborate to achieve a given process. Secondly, the studied SMEs are not necessarily located in the same geographical area as the other nodes of the supply chain. And finally, as a result of the two previous characteristics, SMEs face a lack of visibility in the global supply chain. Thus, the studied supply chain is divided in many sites spread over several geographic locations depending on their purpose or activity in the global supply chain. These sites only have a local visibility but are coordinated with other sites through the product flows. For all these reasons, studying the structure and the behaviour of the supply chain in the SMEs mechatronic field has became a challenge and a growing need was expressed by manufacturers in Savoie.

This paper proposes a modelling solution based on multiagent paradigm. The benefits of multiagent systems (MAS) are widely recognized in literature. Agent technology allows new approach for the modelling and simulation of complex distributed systems. Hence, on one hand, autonomous agents can communicate their preferences, deal objectives with other agents or coordinate together to reach their own objectives or some more global objectives [Bussman et al., 2004]. On another hand, the supply chain is composed by actors or entities which evolve in an organization and interact to achieve a collective purpose. This analogy leads to multiagent approach being a framework naturally oriented to model the supply chain.

To introduce the modelling solution, the first section of the article focuses on the different approaches that were adopted to generate the agentified domain metamodel. Then, we introduce the developed concepts of the supply chain in SMEs context and the multiagent ones and their merger one. In the last section, the dynamic reactive behaviour of the metamodel is introduced before a conclusion is drawn.

APPROACH AND CONCEPTUAL METHODOLOGY

The aim of this paper is to present the application of multiagent system to model the dynamic behaviour of the supply chain in the SMEs context. To reach this purpose, let us first introduce the adopted development

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) process and the conceptual modelling methodology to generate the domain metamodel.

ArchMDE Development Process

ArchMDE (Architecture Model Drinvein Engineering) is a development process proposed within a PhD research work [Azaiez, 2007].

The approach is based on Model-Driven Engineering (MDE) [Kent, 2002] which promoted the separation and combination of models in order to control the software development in its different phases (from the analysis to the implementation). One of the main important issues in MDE approach is the metamodelling one. The metamodel defines the domain concepts, their relationships and their properties. All produced models have to be conform to the metamodel. In our research context, we identify two metamodels related to AchMDE approach. The first one describes properties of functional concepts and **SMEs** Mechatronic supply chain. The second one defines a multiagent metamodel. A combination of the two metamodels will generate an agentified domain metamodel. On the basis of the agentified metamodel, different functional models will be described to introduce the functionalities of the system (Figure 1). Finally, the use of a platform metamodel is necessary to generate the program code.



Figure 1. ArchMDE development process [Tounsi et al., 2009]

In this paper, we describe the first phase of the ArchMDE development process. Therefore, in the following subsections, we introduce the adopted conceptual modelling methodology used to generate the domain metamodel.

Conceptual Modelling Methodology

To identify the concepts and properties of the supply chain in SMEs mechatronic domain, a conceptual methodology is developed. This methodology is an incremental one based on three main visions [Tounsi *et al.*, 2008]: product vision, structure vision and process vision.

In each step, a vision is applied to build or to refine the conceptual model. The result of each step is an intermediary model considered as the input for the next one. Therefore, at the end of the 3 steps, a final architecture of the conceptual model is obtained.

- The Product Vision considers the supply chain • dedicated to a particular product (or a family of a product) from the raw materials to the final goods [Thierry, 2003]. It focuses on the product flow to define the environment and organizations implicated in its management. The environment is characterized by the circulation of the physical flow and the different steps of product transformation as well as the related disturbances. The organizations are entities carrying out one or several activities. In the studied context, the organizations are SME mechatronic that collaborate to accomplish one or several tasks. In our context, the product vision builds the first abstract model of the supply chain.
- The *Structure Vision* has been proposed by Cooper et al. [Cooper *et al.*, 1997]. It considers the architecture of the supply chain composed of: actors (decision-making actors and synchronization actors), network structure (roles in the network and the number of actors in each role) and relationship characteristics between actors. On the basis of the abstract model provided by the previous step, the Structure Vision details the involved organizations and the physical environment. At the end of this step, an intermediary conceptual model is obtained.
- The Process Vision is based on the classification of processes according to the decision-making level [Chopra and Meindl, 2001; Stevens, 1989]: strategic, tactical and operational. While applying Process Vision, various categories of processes are identified and integrated to the previous intermediate model. This can be done according to decision level but also depending on the actors' relationships. These relationships can be classified into two categories: (i) management and control process (ii) synchronization of information and physical flow according to a predefined process scheme. At this last step, a refined conceptual model is generated.



Figure 2. Conceptual Modelling Methodology Framework [Tounsi *et al.*, 2008]

DOMAIN METAMODEL AGENTIFICATION

The first phase of ArchMDE development process consists in the definition and combination of the domain metamodel and multiagent one. Then, main results of this step are outlined in this section. More details can be found in Tounsi et al. [Tounsi *et al.*, 2009].

Domain Metamodel

By applying the proposed conceptual modelling methodology, the main concepts, architecture and processes are identified. The domain metamodel is a representation of these concepts using UML notation (a semi-formal Unified Modelling Language). Each concept is identified through a methodology step. Hence, the final metamodel is depicted in figure 3; each step beings represented in a block.



Figure 3. Domain metamodel

The first block is the group of concepts that are generated in the Product Vision. They define the abstract metamodel composed of:

• *Supply chain (SC)*: this concept defines the root of the domain modelling. All other concepts will detail this concept.

• *Environment*: this concept models the space allocated to the product flow and management through the internal resources as well as the external elements able to influence the activities of the supply chain.

• Sub Supply Chain (SSC): the SSC represents a group of SME which collaborate to achieve an internal aim and/or the overall objective of the supply chain. The SSC is responsible for the management of the product flow in a certain stage of its life cycle.

The application of the Structure Vision results in the refinement of the first abstract model. As outlined in the previous section, these concepts define, on one hand, the network structure according to the decision level, and on the other hand, the actors' type according to their role. Structure vision leads us to identify SSC and Environment architecture. This structure is composed of 3 layers which involve particular concepts and play a specific role:

• The *Monitoring System* models the intelligent layer of the SSC. It controls and monitors the two other layers through the information provided by the Execution System. *Monitoring Actors (MA)* are the main elements of this layer. They model the intelligent actors of SSC and establish metrics to evaluate the performance of the group and consequently act on the two other layers. Therefore, MA are the components responsible for the control and decision-making in SSC but also for the coordination activity in the global supply chain.

• The *Execution System* is the reactive layer of the SSC. It deals with two main roles: (i) it ensures the synchronization of the physical flow according to the information gathered from the *Physical System*, (ii) it observes and corrects the *Physical System* if a perturbation occurs. In abnormal situations, the *Execution System* refers to the *Monitoring System* for coordination and decision-making. *Executive Actors* (*EA*) are the principal entities of this layer. EA mainly models the reactive actors and occasionally MA having reactive behaviour in this layer.

• The *Physical System* is the visible part of the environment from the SSC. It corresponds to the influence perimeter of the SSC. This layer is composed of passive elements controlled by the two other layers of the SSC. Two main concepts are identified: the *Moving Entity (ME)* modelling the product in circulation and the Resource modelling production means.

At the end of this step, an intermediary metamodel is obtained. Finally it's refined by applying the Process Vision. The last block contains these concepts:

• The *Physical Process* (PhP) describes the sequences of processing stages of the product. PhP is a concept to be integrated within a domain metamodel in order to define the tasks that can be handled by the *Execution System*.

• The *Indicator Base* represents a database storing the indicator measures. The EA detects Physical System

deviation according to the gathered information within this database.

• The *Action Base* represents a database that stores the actions to apply when facing an indicator deviation.

• The *Objective* models the global goals of the supply chain or of the SSC ones.

• The *Knowledge Base* represents a database including all knowledge needed by the actors to make the right decision. Knowledge Base can be an organizational knowledge or a constraint.

• The *Organizational Knowledge* is an actor's database that stores information about his acquaintances(others actors in the system).

• The *Constraint* is a variable that an actor must consider to reach the global supply chain goal or the SSC's one.

Thereby, the development of these 3 steps of conceptual modelling methodology, generates a metamodel describing the studied domain regardless the computer technologies. This metamodel is the first artefact of ArchMDE development process.

Multiagent Metamodel

The second artefact to specify concerns the software engineering approach. In this section, we present the multiagent metamodel proposed by Azaiez [Azaiez, 2007] according to the "vowel approach". Indeed, Demazeau [Demazeau, 1996] defines the multiagent system as a set of four main views named "vowel approach":



Figure 4. Multiagent metamodel [Azaiez, 2007]

• Agent view (A): describes the internal structure of an agent. An agent is a computer system able to act autonomously in a given environment in order to meet the design objectives [Wooldridge, 2002]. The scientific community distinguishes three kinds of agent according to their decision-making model and intelligence degree. (i) The reactive agents that react to changes through predefined actions [Brooks, 1991]. (ii) The cognitive agents that have a reasoning faculty and the ability to choose the adequate action in order to achieve an optimal specific goal. This kind of agent also has a learning faculty enabling it to evolve in a decisionmaking system such as BDI agent [Wooldridge, 1999; Bratman et al., 1998]. (iii) The hybrid agent, which is a crossover between the reactive agent and the cognitive agent [Fischer et al., 1995].

• Environment view (E): describes the environment in which evolves the agent. FIPA (Federation of Intelligent Physical Agents) specification defined it as "...all that is external to the agent". According to Azaiez *et al.* [Azaiez *et al.*, 2007b], the environment view can define two different kinds of environment: the simulated one and the deployed one. The simulated environment is a computer representation of an actual environment. It is generally modelled by a metric. The deployed environment deals with computers and appliances in which agents can be deployed, as well as resources that the agent can use. In the context of deployed environments, resources correspond to databases, indicators, variables, etc.

• Interaction view (I): describes the dynamic relationship between agents through protocols or interaction language. This interaction is a structured exchange of messages according to the internal state of the agent and the kind of the interaction framework (coordination, collaboration, cooperation or negotiation).

• Organization view (O): describes the structure of the whole system in terms of agent groups, hierarchy, relationships and the structure of the other entities which constitute the environment.

AEIO approach decomposes the whole multiagent system in several modules. This modularity facilitates the reuse of the different modules according to requirements.

Domain Metamodel Agentification

This step of the ArchMDE methodology consists in merging the multiagent metamodel with the domain one. This combination provides an agentified supply chain metamodel in SMEs field. Hence, a correspondence between the multiagent and the domain concepts is carried out according to their properties and roles in the metamodel. The table 1 summarizes this correspondence.

Table 1	Correspondence between Domain and	
	Multiagent concepts	

Domain concepts	Multiagent concepts
Supply Chain (SC)	MAS
Environment	Environment
Physical System	Resource
Resource	Passive Resource
Moving Entity (ME)	Active Resource
Physical Process (PhP)	Task
Sub Supply Chain (SSC)	Organization
Monitoring System	Group
Execution System	Group
Actor	Agent
Executive Actor (EA)	Reactive Agent with executive role
Monitoring Actor	Cognitive Agent with monitoring
(MA)	and / or coordination role
Objective	Goal
Indicator	Belief
Action	Plan
Knowledge	Knowledge
Organizational	Knowledge
knowledge	_
Constraint	Knowledge

DYNAMIC BEHAVIOUR WITHIN THE SSC'S EXECUTION SYSTEM

The SSC represents a SMEs network collaborating to reach a local objective. In the execution system, the collaborative process takes place in the following scenarios [Tounsi et al., 2009]:

- *Physical system synchronization*: in the "Execution System" of the SSC, actors will synchronize their information and their actions. This collaboration is frequent in the SSC in commonly encountered situations.
- *Physical system control*: the control of the physical system of the SSC will be based on the performance evaluation and the resolution of usual perturbations.

This section describes the reactive dynamic behaviour of the execution system within the SSC through the integration of communication protocols in the agentified domain metamodel. In literature, several protocols extend the Cooperative Problem Solving model (CPS) proposed by Wooldridge and Jennings [Wooldridge and Jennings, 1999]. The CPS defines an abstract way to structure a collective decision-making process in which a group of autonomous agents choose to work together to achieve a common goal. In more details, this model is deployed in four stages:

- Recognition: in which an agent identifies the potential for cooperation.
- Team formation: in which an agent solicits assistance.
- Plan formation: in which the newly formed collective attempts to construct an agreed joint plan.
- Execution: in which members of the collective play out the roles they have negotiated.

The following subsection describes different collaboration processes to implement in the execution system of the proposed metamodel. These protocols follow the CPS abstract model.

Physical Process Synchronization Protocol

According to the metamodel, the Execution system is responsible for the synchronization of the physical process (PhP) in common situations. Indeed, Executive actors (EA) which are reactive agents, synchronise PhP taking into account resources availability. Table 2 summerizes these agentified domain concepts and their role in this protocol.

Table 2. Role of the concepts in physical system synchronization

Domain concepts	Multiagen t equivalent	Role in the protocol
EA	Reactive agent with executive role	EA synchronizes the PhP based on other elements
ME	Active entity	It is the product in circulation. When the PhP ends, the ME sends a synchronization request to the EA with its new state
PhP	Task	It's a task or a physical activity to be handle by the EA
Resource	Passive resource	It is an allocated resource to EA to perform its task.
Organizational	Knowledge	Each EA owns a list that

knowledge	contains information
	about others EA from the
	same SSC. This list
	stores knowledge about
	the name of the EA, the
	task that it performs and
	its resources.

Then, on the basis of these concepts, the synchronization protocol consists of (Figure 5):

- An Executive Agent (EA) receives a request and reacts according to its type. Three kinds of request can be distinguished: a ME request, a collaborative request from another EA or a negative response to a collaborative action initiated by this one.
- If the request is a negative response to a collaborative demand that the EA initiated. In this case, the EA send a request to the coordinator agent of the monitoring system.
- If the request is a synchronization need coming from the Moving Entity (ME) or a collaborative request from another initiator agent, EA checks the availability of the concerned resources.
- If the resource is available, the EA carries out its task, updates the state of ME and informs the other agents from the executive system and the coordinator agent of the end of action.
- If the resource is unavailable and the EA has been solicited by another executive agent to achieve the task, it sends a failure request to the initiator.
- If the resource is unavailable and the EA is in charge of the task then it seeks in its organizational knowledge an agent from the execution system of the SSC that might have the needed resource.
- If the agent finds in its organizational knowledge an agent that can handle the task, it delegates the responsibility of the task. In this case, the collaboration process of the concerned agent will be activated and follows the same sequence.
- If the agent does not find another agent having the needed resource to handle the task, it sends a request to the coordinator agent. This agent is a monitoring agent (MA) that receives requests from Execution System. MA diffuses the information to other monitoring agents of the SSC in order to find a solution.



Figure 5. EA Behavior

Physical System Control Protocol

This protocol is based on performance evaluation. At the physical process synchronization end, each EA updates the indicators values that evaluate the performance of its activity and related resources. Then, the table 3 summarises the different concepts and their role in the control process.

According to the table 3, the behaviour of involved concepts constitutes the "Control physical system process":

- At the end of its synchronization task, the EA evaluates the performance of its activity and related resources (the allocated space of the environment to the EA).
- According to this perception, the EA refers to the indicator base in order to detect a perturbation.
- If the EA finds an indicator deviation, it seeks the cause of the perturbation.
- If the deviation is a common situation, the EA selects the appropriate action plan to solve the problem and applies it to the environment.
- If a new situation occurs, the EA sends a failure control message to the coordinator MA. Then, the MA spreads the information in the monitoring system.

Table 3. Role of concepts in physical control protocol

Domain	Multiagent	Role
concepts	concepts	
EA	Reactive	EA evaluates the
	agent with	performance of the
	executive	physical system and
	role	acts on it
		consequently
Indicator	Belief	Belief of agent about
		the optimal
		performance state of
		the environment
Action	Plan	A reactive plan
		established by the
		monitoring system.
		EA reacts to the
		perception from the
		environment
		according to the plan
Environment	Environmen	It is the allocated
	t	space to the EA to
		act on it
MA	Cognitive	MA receives the
	agent with a	failure message from
	coordinator	the EA when an
	role	uncommon
		perturbation occurs

The figure 6 describes the sequence diagram of the "Physical Process Control" using UML formalism.



Figure 6. Sequence Diagram of Physical process control

CONCLUSION

This article presents a metamodel describing the supply chain in the SMEs mechatronic context. Our approach combines this domain metamodel (scope of research) to the multiagent one based on the ArchMDE development process. This process allows the separation of the architecture building and the study of the concepts behaviour based on multiagent paradigm in order to facilitate and control the software development. This work describes how to generate the domain metamodel, the multiagent one and the merging one. Then, on the basis of the obtained concepts, we propose two processes in order to synchronize and control dynamically the physical flow. There are a number of issues that we intend to address in future work, the most direct of which is the implementation of a collaborative process in the monitoring layer (intelligent layer of the SSC) and coordination processes between different SSC that constitute the global supply chain.

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A MULTI-AGENT MODEL FOR MUTUAL ABSORPTION OF EMOTIONS

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Emotion Contagion, Social Simulation, Analysis.

ABSTRACT

In recent times researchers have initiated investigating emotion as a collective property of groups, emphasizing the influence of combined emotions among group members on group processes. Within groups humans recognize and react emotionally to expressions of emotions of other group members. This paper uses a multi-agent-based approach to formalize and simulate such emotion contagion within groups.

INTRODUCTION

Within psychology, emotion is often defined as a state or process that plays a role in various cognitive processes, among which decision making and action preparation. Emotions are elicited by a particular stimulus, often include physiological reactions, and are relatively intense and short-lived (Frijda 1986). In addition, emotions have a social function: humans may experience situations where expressions of emotion by one individual shape the emotions, thoughts and behavior of others; others' reactions can then influence their future interactions with the individual expressing the original emotion, as well as that individual's future emotions and behaviors; e.g. (Hareli, Rafaeli 2008), (Hatfield, Cacioppo, Rapson 1994). This everyday, continuous, automatic process of emotion contagion has been described as a tendency to mimic the nonverbal behavior of others, to "synchronize facial expressions, vocalizations, postures, and movements" with others, in order to "converge emotionally" (Hatfield, Cacioppo, Rapson 1994).

Modeling group emotion can be done at the level of the group or at the level of the individuals, which has been named respectively the top-down and bottom-up approach (Barsade, Gibson 1998). The bottom-up perspective sees group emotion as the sum of its parts, affected by the homogeneity or heterogeneity of the group and the mean emotions of the group members. Individual differences play an important role, such as specific personality traits and the underlying brain mechanisms. There is consensus that the basic structure of personality incorporates five superordinate factors (McCrae, Costa 1987): extraversion, agreeableness, conscientiousness, emotionality and intellect. Extraversion is characterized as a tendency towards sociability. activeness. dominance and craving excitement. Agreeableness is thought of as being concerned with the maintaining of relationships. Conscientiousness reflects qualities of planning, persistence, and purposeful striving towards goals. Emotionality (or neuroticism) concerns the ease and frequency with which a person becomes upset and distressed. Intellect (or openness) reflects openness to experience and intelligence-related sub-traits such as creativity and curiosity. Personality intellect, dimensions have been linked to specific aspects of brain functioning. The functional approach considers two sets of structures in the brain, the behavioral approach system (BAS), and behavioral inhibition system (BIS) (Grav 1990). BAS causes animals and humans to move towards incentives: things they desire. Besides managing the approach, BAS also creates excitement and positive feelings (Carver, Scheier 2004). The system BIS can be thought of as a stopping system, a system responsive to threat. BIS is responsive to cues of punishment and danger, not incentives. The neurotransmitter linked to BIS is serotonin (Gray 1990). The feeling BIS creates is anxiety. The two systems have been linked with personality traits: BIS is critical to neuroticism and BAS to extraversion (seeking social incentives) (Carver, Scheier 2004).

Personality also has been related to the functioning of the nervous system in a variable called sensation seeking (Zuckerman 1994). People who score high on sensation seeking are in search for new and exciting experiences. They are more likely to do high-risk sports, such as skydiving, are more sexually experienced and sexually responsive and compared to people low on this trait, are faster drivers. Zuckerman (Zuckerman 1994) has suggested that there is a particular brain chemical for sensation seeking (an enzyme called monoamine oxidase. MAO), which regulates several neurotransmitters, including serotonin and dopamine. Sensation seeking has also been related to the previously mentioned BIS and BAS systems (Carver, Scheier 2004). Persons high on sensation seeking correspond to a high BAS and low (sensitive) BIS.

In the literature, the area of emotion contagion in groups has been studied from the theoretical side (Barsade, Gibson 1998) but no computational models of emotion contagion have been developed. This paper is an attempt to develop a computational model of emotion contagion in groups incorporating the concepts given in the literature. The goal of this paper is to introduce a multi-agent-based modeling approach that formalizes and simulates the dynamics of emotion contagion within groups. The proposed approach makes use of standard numerical simulation software for simulation purposes, and the high-level declarative temporal modeling language TTL (Bosse, Jonker, Meij, Sharpanskykh, Treur 2008) for analysis purposes. This modeling language is well suited for the current purposes, since it allows the modeler to combine qualitative, logical aspects with quantitative, numerical aspects (such as real numbers, and mathematical operations).

In the next section a detailed model of group emotion contagion is explained and formalized. In the section after that, simulation results are presented. Thereafter a section is devoted for mathematical analysis. Furthermore, the section thereafter addresses formal verification of the emotion contagion model and the simulation results. Finally the last section concludes the paper with a discussion.

A MULTI-AGENT EMOTION ABSORPTION MODEL

The model introduced in this paper has been designed as an interpretation of the bottom-up approach where group emotion can be seen as the sum of its parts (Barsade, Gibson 1998); therefore it is named absorption model¹. It distinguishes multiple factors that influence emotion contagion processes. The model incorporates individual differences in personality traits (McCrae, Costa 1987): neuroticism and extraversion (BIS and BAS, (Gray 1990)). A number of aspects of the proposed computational model are distinguished that play a role in the contagion, varying from aspects related to an agent *S* sending the emotion, an agent *R* receiving the emotion, and the channel between sender *S* and receiver *R*; see Table 1.

Table 1 Aspects related to a sender *S*, receiver *R*, or both

level of the sender's emotion	
level of the receiver's emotion	q_R
sender's emotion expression	\mathcal{E}_S
openness for received emotion	δ_{R}
the strength of the channel from sender to receiver	α_{SR}

The aspect ε_S depends on how introvert or extravert, expressive, and/or active or energetic the person is. These aspects correspond to the personality trait extraversion and sensation seeking and the underlying neural system BAS. It represents in how far a person transforms internal emotion into external expression. In this sense, an introvert person will induce a weaker contagion of an emotion than an extravert person. The aspect α_{SR} depends on the type and intensity of the contact between the two persons (e.g., distance vs attachment). The aspect δ_R indicates the degree of susceptibility of the receiver. This represents in how far the receiver allows the emotions received from others to affect the own emotion, and how flexible/persistent the person is emotionally.

The parameter α_{SR} may be related to a combination of more specific aspects such as the directness of the emotion contagion, and the relations between sender and receiver. Emotion contagion is direct if the persons infecting each other with emotions are together in the same room and pay attention to each other (Hareli, Rafaeli 2008). Indirect contagion can happen when for instance the contagion between others is observed. Direct contagion is propagated stronger than indirect emotion contagion.

The aspects shown in Table 1 have been formalized numerically by numbers in the interval [0, 1]. In addition, the parameter γ_{SR} is used to represent the strength by which an emotion is received by R from sender *S*, modeled as: $\gamma_{SR} = \varepsilon_S \alpha_{SR} \delta_R$. The stronger the channel, the higher α_{SR} and the more contagion will take place. The model works as follows: if γ_{SR} is θ , there will be no contagion, if it is I, there will be a maximum strength of contagion. If γ_{SR} is not θ , there will be contagion and the higher the value, the more contagion will take place. In a way γ_{SR} expresses the energy level with which an emotion is being expressed, transferred and received. The overall strength by which emotions from all the other group members are received by R in a group G, indicated by γ_R , is defined as $\gamma_R =$ $\Sigma_{S \in G \setminus \{R\}}$ γ_{SR} . Suppose G is a group of agents. Take weights proportional to $\varepsilon_S \alpha_{SR}$ defined by $w_{SR} = \varepsilon_S \alpha_{SR} / \omega_{SR}$ $\Sigma_{C \in G \setminus \{R\}} \in \mathcal{E}_C \alpha_{CR}$ and for any $R \in G$ let $q_R^* = \Sigma_{S \in G \setminus \{R\}} w_{SR} q_S$ be the weighted combined emotion from the other agents. The set of differential equations for emotion contagion in group G is

$$dq_R/dt = \gamma_R \left(q_R^* - q_R \right)$$

for all $R \in G$. Here $\gamma_R = \sum_{S \in G \setminus \{R\}} \gamma_{SR}$ with $\gamma_{SR} = \varepsilon_S \alpha_{SR} \delta_R$.

SIMULATION RESULTS

A large number of simulations have been performed, using standard numerical simulation software, resulting in a variety of interesting patterns. In this section some of the simulation results are discussed. More simulation results can be found in Appendix A at http://www.few.vu.nl/~tbosse/emotion/ECMS09.pdf.



Figure 1. Simulation trace 1 (all $\gamma_R = I$)

¹ Note that it is not claimed that this model can describe the emotional dynamics of all persons in all situations. For some situations, an "amplification approach" seems to be more appropriate (see section about discussion).

The next section presents results of a mathematical analysis; the occurrence of most patterns under certain conditions was proven. Simulations shown here are for a group of 3 agents. A first pattern found is that when the γ_R for all agents are not θ , in this case they are all I, the emotion levels of all of them will approximate their average initial emotion level, with speed depending on the δ_R (susceptibility) and $\varepsilon_S \alpha_{SR}$; see Figure 1. The occurrence of this pattern has been proved mathematically; see Theorem 3 in the next section.



The opposite of this pattern happens when all γ_R are θ , then all agents will have equilibria that are equal to their initial emotional levels. In other words: the emotional levels of all agents will not change at all; see Theorem 1 in the next section. Another situation (see Figure 2) occurs when agent a has δ_a set to θ and the other agents have this parameter $\neq 0$. This situation represents that agent a is not open to receive emotions, but can send emotions. As a result agent a's initial emotion level will remain the same. Furthermore, the agents b and c will eventually reach the equilibrium of agent a, which is equal to his initial emotion level.



Figure 3. Simulation trace 3 ($\delta_R(a, b, c) = (0, 0, 0.5)$)

In Figure 3 it is shown that when agent a and b both have δ_R set to θ , agent c will reach a value in between a and b's initial emotion values. The actual value agent c reaches depends on the settings of the parameter settings for all agents. This situation represents a case where two agents do not change their emotional level because they are only open to sending emotions, but not receiving emotions. As a result the third agent is forced to reach a value in between the emotional levels of the others. A next situation (see Figure 4) is one where δ_a and ε_a are set to θ . This represents agent a being bidirectionally excluded form emotion contagion: (s)he can not receive or send emotions. The agents b and c are forced to go to a certain average in between their initial emotion values. The exact value they reach depends on the settings of their δ_R (susceptibility) and $\varepsilon_S \alpha_{SR}$.



MATHEMATICAL ANALYSIS

This section presents some of the results of a mathematical analysis of the model that has been made. Note that $\gamma_A = 0$ iff $\sum_{B \in G \setminus \{A\}} \varepsilon_B \alpha_{BA} \delta_A = 0$ iff $\varepsilon_B \alpha_{BA} \delta_A = 0$ for all $B \neq A$. This means that $\gamma_A = 0$ can only occur when for each $B \neq A$ either $\varepsilon_B = 0$ or $\alpha_{BA} = 0$ or $\delta_A = 0$. This can be interpreted in the sense that A is isolated from emotional impact of all group members. In such a special case q_A will always be in an equilibrium state.

Theorem 1 (No change when $\gamma_A = \theta$)

If $\gamma_A = 0$ then the emotion value for A will be in an equilibrium right from the start.

Next, conditions on monotonicity are addressed. Assuming $\gamma_A > 0$, from the equations it follows that $dq_A/dt \ge 0$ if and only if $q_{A^*} \ge q_A$. In particular, for A with the lowest q_A it holds $q_B \ge q_A$ for all $B \ne A$, and therefore via $q_{A^*} = \sum_{B \in G \setminus \{A\}} w_{BA} q_B \ge \sum_{B \in G \setminus \{A\}} w_{BA} q_A = q_A$ it follows that q_A is monotonically increasing. Similarly the highest q_A is monotonically decreasing.

Theorem 2 (Monotonicity Conditions)

Suppose $\gamma_A > 0$. Then the following hold:

- (a) q_A is monotonically increasing iff $q_{A^*} \ge q_A$ q_A is strictly monotonically increasing iff $q_{A^*} > q_A$
- (b) q_A is monotonically decreasing iff $q_{A^*} \le q_A$ q_A is strictly monotonically decreasing iff $q_{A^*} < q_A$
- (c) If q_B ≥ q_A for all B ≠ A, then q_A is monotonically increasing.
 If in addition q_B > q_A for at least one B ≠ A, then q_A is strictly increasing.
- (d) If q_B ≤ q_A for all B ≠ A, then q_A is monotonically decreasing.
 If in addition q_B < q_A for at least one B ≠ A, then q_A is strictly decreasing.

Next, equilibria are addressed for $\gamma_A > 0$. When at some point in time all q_A are the same, then from Theorem 2(c) and (d) it follows that they are both (non-strictly) monotonically increasing and decreasing, so they are in an equilibrium. Moreover, from Theorem 2(c) and (d) it follows that as long as the values of the q_A are different, then the lowest and highest values keep on changing (strictly increasing, resp. decreasing), so are not in an equilibrium. This implies the following identification of equilibria.

Theorem 3 (Equilibria when $\gamma_A > \theta$ for all A)

Suppose $\gamma_A > 0$ for all A. Then the equilibria are the cases where all q_A are equal. Equilibria are reached between the lowest and highest initial value.

In some cases the equilibria are the average of the initial values, due to preservation of the (overall) sum of the emotion levels: $\sum_{A \in G} q_A(t') = \sum_{A \in G} q_A(t)$ for all t and t' or $\sum_{A \in G} q_A(t + \Delta t) = \sum_{A \in G} q_A(t)$ for all *t* and Δt .

Taking the sum of the equations, the criterion for preservation is

 $\Sigma_{A \in G} \gamma_A (q_{A^*} - q_A) = 0$ or $\Sigma_{A \in G} \gamma_A q_{A^*} = \Sigma_{A \in G} \gamma_A q_A$ Now

 $\gamma_A w_{BA} = \sum_{C \in G \setminus \{A\}} \gamma_{CA} w_{BA} = \sum_{C \in G \setminus \{A\}} \varepsilon_C \alpha_{CA} \delta_A w_{BA}$

$$= (\Sigma_{C \in G \setminus \{A\}} \ \mathcal{E}_C \ \alpha_{CA}) \ \partial_A \ \mathcal{E}_B \ \alpha_{BA} / \Sigma_{C \in G \setminus \{A\}} \ \mathcal{E}_C \ \alpha_{CA}$$

 $= \varepsilon_B \alpha_{BA} \delta_A = \gamma_{BA}$

Therefore

 $\gamma_A q_{A^*} = \sum_{B \in G \setminus \{A\}} \gamma_A w_{BA} q_B = \sum_{B \in G \setminus \{A\}} \gamma_{BA} q_B$ and taking the sum

 $\sum_{A \in G} \gamma_A q_{A^*} = \sum_{A \in G} \sum_{B \in G \setminus \{A\}} \gamma_{BA} q_B =$

 $\Sigma_{B \in G} \Sigma_{A \in G \setminus \{B\}} \gamma_{BA} q_B = \Sigma_{B \in G} (\Sigma_{A \in G \setminus \{B\}} \gamma_{BA}) q_B$ It follows that the criterion for overall emotion preservation is equivalent to

 $\Sigma_{A \in G \setminus \{B\}} \ \gamma_{BA} = \ \gamma_B = \ \Sigma_{A \in G \setminus \{B\}} \ \gamma_{AB}$ for all *B* which in terms of the basic parameters is equivalent to for all *B*.

 $\Sigma_{A \in G \setminus \{B\}} \varepsilon_B \alpha_{BA} \delta_A = \Sigma_{A \in G \setminus \{B\}} \varepsilon_A \alpha_{AB} \delta_B$

Theorem 4 (Preservation of overall emotion)

The following are equivalent:

- (i) The overall emotion in the group is preserved
- (ii) $\sum_{A \in G \setminus \{B\}} \gamma_{BA} = \sum_{A \in G \setminus \{B\}} \gamma_{AB}$ for all *B*.
- (iii) $\sum_{A \in G \setminus \{B\}} \varepsilon_B \alpha_{BA} \delta_A = \sum_{A \in G \setminus \{B\}} \varepsilon_A \alpha_{AB} \delta_B$ for all *B*.

When these conditions are satisfied, an equilibrium is reached where each emotion level is the average of the initial emotion levels.

The conditions are satisfied in particular when all γ_{BA} are equal, or when, more specifically, all ε_A are equal, all α_{AB} are equal and all δ_B are equal.

Finally it is analyzed under which conditions the emotion values stay within the interval [0, 1] (closure property). It can easily be verified that the expression describing change reaches its maximum for $\varepsilon_A = \alpha_{AB} =$ $\delta_B = q_S = 1$ and $q_R = 1$. Similarly, this function reaches its minimum for $\varepsilon_A = \alpha_{AB} = \delta_B = q_R = 1$ and $q_S = 0$. Using this the following equations for upper and lower bounds are obtained:

 $(1 - (\#(G) - 1))\Delta t = q_{min} \le q_R(t + \Delta t) \le q_{max} = (\#(G) - 1)\Delta t$ In order to maintain the closure property for emotion contagion in the absorption model, q_{max} has to be constrained to 1 and q_{min} to 0. Therefore, respectively:

 $(\#(G)-1).\Delta t \le 1 \text{ and } (1-(\#(G)-1))\Delta t \ge 0$

which both lead to the same constraint $\Delta t \leq 1/(\#(G) - 1)$. So, as long as this constraint is maintained, the closure property holds for the absorption model:

Theorem 5 (Closure property)

The emotion values generated remain in the interval [0, 1] if $\Delta t \leq 1/(\#(G) - 1)$.

FORMAL VERIFICATION

This section addresses analysis of the emotion contagion model by verification of dynamic properties. The purpose of this type of verification is to check whether the model behaves as it should. A typical example of a property that may be checked is whether no unexpected situations occur, such as a variable running out of its bounds (e.g., $q_A(t) > 1$, for some t and A), or whether eventually an equilibrium value is reached. Other, more complex examples can be found in the theorems presented in the previous section. To analyze the resulting simulation traces in more detail, the TTL Checker tool (Bosse, Jonker, Meij, Sharpanskykh, Treur 2008) has been used. This tool takes as input a temporal predicate logical language TTL formula and a set of traces, and verifies automatically whether the formula holds for the traces. TTL is built on atoms referring to states of the world, time points and traces, i.e. trajectories of states over time. In addition, dynamic properties are temporal statements that can be formulated with respect to traces based on a state ontology. For the emotion absorption model, a number of such dynamic properties have been formalized in TTL varying from properties addressing limit behavior (equilibria reached) to properties of the process from initial values to the equilibria. Below, a number of these properties are introduced, both in semiformal and in informal notation (where state(γ , t) |= p denotes that p holds in trace γ at time t). Note that the properties are all defined for a particular trace γ and sometimes for a particular time interval between tb and te.

P1a - Emotional Stability for Agent a

For all time points t1 and t2 between tb and te in trace γ , if at t1 the level of emotion of agent a is x1, then at t2 the level of emotion of agent a is between x1 - α and x1 + α . P1a(γ :TRACE, tb, te:TIME, a:AGENT, α :REAL) =

∀t1,t2:TIME ∀x1,x2:REAL

state(γ, t1) |= emotion(agent(a), x1) &

state(y, t2) |= emotion(agent(a), x2) &

 $tb \leq t1 \leq te \ \& \ tb \leq t2 \leq te \Rightarrow x1\text{-}\alpha \leq x2 \leq x1\text{+}\alpha$

This property can be used to verify in which situations a certain agent's level of emotion does not fluctuate much. It has been found, for example, that for the trace shown in Figure 1 and for $\alpha = 0.00001$, the emotion of agent a remains stable between time point 28 and 50. In

other words, checking P1a(traceFig1, 28, 50, a, 0.00001) was successful, where traceFig1 is the trace of Figure 1.

P1b - Emotional Stability for Agent a around Value x

For all time points t between tb and te in trace γ

the level of emotion of agent a is between x - α and x + α (where α is a constant).

P1b(γ :TRACE, tb, te:TIME, x:REAL, a:AGENT, α :REAL) = \forall t:TIME \forall y:REAL

state(γ , t) = emotion(agent(a), y) & tb \leq t \leq te \Rightarrow x- $\alpha \leq$ y \leq x+ α

As a variant of P1a, property P1b can be used to check whether an agent's level of emotion stays around a certain (given) value. For example, for $\alpha = 0.0001$, property P1b(traceFig1, 25, 50, 0.4333, b, 0.0001) was true. One step further, P1a and P1b can be used as building blocks to check the propositions and theorems related to equilibria presented in the previous section against the generated traces. For example, property P1c checks whether Theorem 3 holds:

P1c - Equal Equilibria

If for all agents A and B, γ_{AB} is nonzero in trace γ then eventually the same equilibrium q (between 0 and 1) will occur for all agents P1c(γ :TRACE, α :REAL) =

[\forall a1,a2:AGENT [a1≠a2 \Rightarrow ∃g:REAL>0

 $[state(\gamma, 1) |= has_gamma_for(agent(a1),agent(a2),g)]]]$ $\Rightarrow [\exists q:REAL \forall a:AGENT P1b(\gamma,40,50,q,a, \alpha)]$

This property, which has been proven in the mathematical analysis, has been checked for $\alpha = 0.07$ for all generated traces, and indeed was confirmed. In addition, similar properties have been formulated that make claims about the equilibria on the basis of the initial settings. Due to space limitations, details of these properties are not shown here. However, some examples (in informal notation) are:

- In case $\gamma_{SR} = 0$ for all agents, then each agent ends up in an equilibrium that is equal to its initial emotion value.
- In case $\delta_R = 0$ for exactly 1 agent A (i.e., $\delta_A = 0$), and other δ_R are nonzero, and all α_{SR} and ε_S are nonzero for all agents, then each agent ends up in an equilibrium that is equal to the initial emotion value of agent A.
- In case $\delta_R = 0$ and $\varepsilon_S = 0$ for exactly 1 agent A (i.e., $\delta_A = \varepsilon_A = 0$), and other δ_R and ε_S are nonzero, and all α_{SR} are nonzero for all agents, then agent A ends up in an equilibrium that is equal to its initial emotion value, and all other agents end up in an equilibrium that is in between their initials emotion values.
- In case $\delta_R = 0$ for exactly 2 agents A and B (i.e., $\delta_A = \delta_B = 0$), and other δ_R are nonzero, and all α_{SR} and ε_S are nonzero for all agents, then agent A and B end up in an equilibrium that is equal to their initial emotion value, and all other agents end up in an equilibrium that is in between the initial emotion values of A and B.

P2a - Monotonic Increase of Emotion²

For all time points t1 and t2 between tb and te in trace γ , if at t1 the level of emotion of agent a is x1, and at t2 the level of emotion of agent a is x2 and t1 < t2, then x1 ≤ x2. P2a(γ :TRACE, tb, te:TIME, a:AGENT) = \forall t1,t2:TIME \forall x1,x2:REAL $\begin{array}{l} \mbox{state}(\gamma,\,t1) \mid = \mbox{emotion}(\mbox{agent}(a),\,x1) \ \& \\ \mbox{state}(\gamma,\,t2) \mid = \mbox{emotion}(\mbox{agent}(a),\,x2) \ \& \\ \mbox{tb} \leq \mbox{t1} \leq \mbox{te} \ \& \mbox{tb} \leq \mbox{t2} \geq \mbox{te} \ \& \mbox{t1} < \mbox{t2} \Rightarrow \mbox{x1} \leq \mbox{x2} \end{array}$

Property P2a and the variant P2b addressing monotonic decrease (by replacing \leq in the consequent by \geq) can be used to check whether an agent's level of emotion increases or decreases monotonically over a certain interval. Such monotonicity, for example, occurs for agent c during the whole trace shown in Figure 1 (i.e., property P2b(traceFig1, 1, 50, c) succeeded). Furthermore, these properties can be used as building blocks to check the propositions and theorems related to monotonicity presented in the previous section against the generated traces. For example, property P2c checks whether part (c) and (d) of Proposition 1 hold:

P2c - Conditional Monotonicity

For all agents A, if $q_{A^*} \ge q_A$ between tb and te in trace γ , then q_A is monotonically increasing during this interval, and if $q_{A^*} \le$ q_A between tb and te in trace γ , then q_A is monotonically decreasing during this interval. P2c(γ :TRACE, tb, te:TIME) = ∀a1:AGENT [[∀t:TIME ∃a2,a3:AGENT ∃x1,x2,x3,w2,w3:REAL state(γ , t) |= emotion(agent(a1), x1) & state(γ , t) |= emotion(agent(a2), x2) & state(γ , t) |= emotion(agent(a3), x3) & a2 \neq a3 & tb \leq t \leq te & state(\u03c7, 1) |= has_w_for(agent(a2),agent(a1),w2) & state(\u03c7, 1) |= has_w_for(agent(a3),agent(a1),w3) & $w2^{*}x2+w3^{*}x3 \ge w1] \Longrightarrow p2a(\gamma, tb, te, a1)] \&$ [[∀t:TIME ∃a2,a3:AGENT ∃ x1,x2,x3,w2,w3:REAL state(γ , t) |= emotion(agent(a1), x1) & state(γ , t) |= emotion(agent(a2), x2) & state(γ , t) |= emotion(agent(a3), x3) & a2 \neq a3 & tb \leq t \leq te & state(\u03c7, 1) |= has_w_for(agent(a2),agent(a1),w2) & state(γ, 1) |= has_w_for(agent(a3),agent(a1),w3) &

 $w2^{*}x2+w3^{*}x3 \leq w1] \Longrightarrow p2b(\gamma, tb, te, a1)]$

Here, q_{al*} is explained in the section after the introduction section. This property has been confirmed for all possible intervals in all generated traces.

P3 - Emotion between Boundaries

For all time points t between tb and te in trace γ if at t the level of emotion of agent a is x, then min < x < max. P3(γ :TRACE, tb, te:TIME, max, min:REAL, a:AGENT) = \forall t:TIME \forall x:REAL

 $state(\gamma, \, t) \mid = emotion(agent(a), \, x) \ \& \ tb \leq t \leq te \Rightarrow min \leq x \leq max$

This property can be used to check whether the emotion of an agent stays between certain boundaries. For example, no emotional value should ever become lower than 0 or higher than 1. This turned out to be the case for all generated traces where $\Delta t \leq 1/(\#(G) - I)$. That is, property P3(trace, 1, 50, 0.0, 1.0, X) succeeded for all traces trace with these settings and agents X, which confirms Theorem 5 of the previous section. In addition, it was found that the property failed for some traces that do not have these settings. E.g., for a trace with $\Delta t = 0.7$, all $\gamma_{SR} = 1$, and initial values $q_A = 0.3$, $q_B = 0.1$, and $q_C =$ 0.9, the emotion values eventually run out of their boundaries.

² A strict variant of such properties can be created by replacing \leq by <.

P4 - Emotion Agent a1 above Agent a2

For all time points t between tb and te in trace γ , if at t the level of emotion of agent a1 is x1 and the level of emotion of agent a2 is x2, then x1 \geq x2. P4(γ :TRACE, tb, te:TIME, a1, a2:AGENT) = \forall t:TIME \forall x1,x2:REAL state(γ , t) |= emotion(agent(a1), x1) & state(γ , t) |= emotion(agent(a2), x2) & tb \leq t \leq te \Rightarrow x1 \geq x2

Property P4 can be used to check whether an agent's emotion level stays above (or below) another agent's level during a specified interval. For example, in the trace of Figure 1, agent c always has a higher emotion than agent a (i.e., property P4(traceFig1, 1, 50, c, a) succeeded). However, in the end the difference becomes very small, and if the simulation were continued longer, eventually this property would fail.

P5 - Emotion Approaches Value x with Speed s

For all time points t1 and t2 between tb and te in trace γ , if at t1 the level of emotion of agent a is x1, and at t2 the level of emotion of agent a is x2, and t2 = t1+1, then s * $|x-x1| \ge |x-x2|$ (where s is a constant < 1).

 $\begin{array}{l} \mathsf{P5}(\gamma:\mathsf{TRACE}, tb, te:\mathsf{TIME}, x:\mathsf{REAL}, a:\mathsf{AGENT}) \equiv \\ \forall t1, t2:\mathsf{TIME} \ \forall x1, x2:\mathsf{REAL} \\ \text{state}(\gamma, t1) \mid = emotion(agent(a), x1) \ \& \\ \text{state}(\gamma, t2) \mid = emotion(agent(a), x2) \ \& \\ tb \leq t1 \leq te \ \& tb \leq t2 \leq te \ \& t2 = t1+1 \Rightarrow |x-x1| \ * \ s \geq |x-x2| \end{array}$

Property P5 can be used to check whether an agent's emotion level approaches a given value x, and to determine the speed s with which this happens (where 0 < s < 1, and a high s denotes a slow speed). For example, for the trace shown in Figure 2, it turned out that agent b approaches emotion level 0.3 with a speed of approximately 0.9991.

DISCUSSION

Usually computational models of emotion consider a single agent (Gratch, Marsella 2001). However, since a couple of decades, researchers have started to investigate emotions as a collective property of groups, emphasizing the influence of collective emotions among group members on group processes (Barsade, Gibson 1998). Inspired by these developments, the current paper proposed a multi-agent-based approach to formalize and simulate the dynamics of emotion absorption within groups. In contrast to most existing (symbolic) agent-based modeling approaches, the current approach represents a multi-agent system using numerical techniques. A dynamical systems style multiagent model has been developed and simulated. Although an extensive empirical validation is left for future work, these experiments pointed out that the model is able to produce various interesting emerging patterns as described (informally) in the psychological literature. Moreover, by a mathematical analysis a number of properties of the model have been determined, among which conditional monotonicity properties and the occurrence of equilibria. Using the TTL checking software, several of these properties have been verified and confirmed against generated simulation traces, which is an important additional indication that the model behaves as expected. As a next

step, a more detailed validation of the model in laboratory experiments is planned. The idea is to create a setting in which various humans interact in a room, while continuously being subject to (physiological) measurements (e.g., using emotion recognition approaches as discussed in (Goldman, Sripada 2005)) to assess their emotion. The obtained data can then be used to fine-tune the model.

Concerning further work, other possible models are being examined as well. For instance, another model of emotion contagion could represent patterns where emotion is amplified through contagion instead of being absorbed as in the current model. This amplification model could correspond to so called upwards and downwards emotional spirals that are hypothesized by the authors in (Frederickson, Barbara, Joiner, Thomas 2002), based on Frederickson's broaden-and-build theory. A corresponding personality trait that could model this difference between absorbing or amplifying emotions in the emotion contagion process could be the 'sensation seeking' personality trait (Zuckerman 1994).

Besides extending the presented model or examining other models, it is worthwhile to investigate the possibilities to apply it in real-world case studies. An interesting application is to exploit it in an Ambient Intelligence setting. The idea is to develop an Ambient Agent that is able to estimate the group emotion of a team in a particular environment (e.g., a team of operators on a naval vessel, or a sports team), and to provide support in case the group emotion negatively affects the team performance. This direction will be further explored in future research.

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ECOSIMNET: A FRAMEWORK FOR ECOLOGICAL SIMULATIONS

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ABSTRACT

Simulating ecological models is always a difficult task, not only because of its complexity but also due to the slowness associated with each simulation run as more variables and processes are incorporated into the complex ecosystem model. The computational overhead becomes a very important limitation for model calibration and scenario analysis, due to the large number of model runs generally required. This paper presents a framework for ecological simulations that intends to increase system performance through the ability to do parallel simulations, allowing the joint analysis of different scenarios. This framework evolved from the usage of one simulator and several agents, that configure the simulator to run specific scenarios, related to possible ecosystem management options, one at a time, to the use of several simulators, each one simulating a different scenario concurrently, speeding up the process and reducing the time for decision between the alternative scenarios proposed by the agents. This approach was tested with a farmer agent that seeks optimal combinations of bivalve seeding areas in a large mariculture region, maximizing the production without exceeding the total allowed seeding area. Results obtained showed that the time needed to "near" optimal solution acquire а decreases proportionally with the number of simulators in the network, improving the performance of the agent's optimization process, without compromising its rationality. This work is a step forward towards an agent based decision support system to optimize complex environmental problems.

INTRODUCTION

Ecological models are simplified views of nature, used to solve scientific and/or management problems. These models can be seen as geographical maps (which themselves can be seen as models) - different types of maps serve different purposes: for cars, for railways, for airplanes, for pedestrians, for geologists, and so on. They focus on different objects, so they have different layouts and they exist also in different scales intending to be used in different applications. Pedro Duarte CIAGEB – UFP, University Fernando Pessoa Praça 9 de Abril, 349, 4249-004 Porto, Portugal E-mail: pduarte@ufp.edu.pt

Ecological models contain only the characteristic features that are essential in the context of the problem to be solved or described. They may be considered a synthesis of what is known about the ecosystem with reference to the considered problem. As opposed to a statistical analysis based on empirical relationships between the data, a model is able to translate the modeller's knowledge about a system, formulated in mathematical equations and component relationships (Jørgensen and Bendoricchio 2001). For the same ecosystem there may be different ecological models, selected in accordance to the model's goals.

Coastal ecosystems always played an important role in the life of human beings. They allow an enormous amount of possible activities (such as fishing, aquaculture, harbour activities, tourism, etc.), and guarantee several basic services to humanity, but they are also the final destination of many pollutants generated by agriculture and other human activities (Duarte et al. 2007). In the last century, human population migrated intensively from inland to coastal boundaries and, nowadays, the World Bank estimates that 50% of the world's population lives within 60km from the sea (Watson et al. 1996). These numbers are more relevant in Portugal where almost 89% of the population lives within 50km from the sea and occupies only 39% of the territory (INE 2008). The occurrence of ecological disasters alerted the scientists and stakeholders to the need of working together towards the sustainable management of coastal ecosystems within the framework of Integrated Coastal Zone Management programs.

Realistic simulations of coastal ecosystems require describing several physical, chemical and biological processes in mathematical terms. Physical processes include flow and circulation patterns, mixing and dispersion of mass and heat, settling and resuspension of planktonic organisms and suspended matter, solar radiation and light penetration. Chemical processes include biogeochemical cycles of important elements, such as nitrogen and phosphorus. Biological processes include growth and death rate of any organisms that may alter the concentration of different elements. The accurate simulation of these processes is very important for setting up a realistic model of the whole ecosystem. Detailed representations of these processes can be found in the literature since the 1980's (Jørgensen and Bendoricchio 2001).

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) When coastal ecosystems are exploited for shellfish aquaculture one of the issues that always arises is how far the holders can increase the production in their assets without exceeding ecosystem carrying capacity (Duarte et al. 2003). Usually, the balance is maintained by legislation, which limits the areas of exploitation and thus the number of licenses in each area. Stakeholder's experience, usually acquired by trial and error, successes and failures, leads them to have an empirical perception of what is the optimal exploitation density of each species per unit area, without much consideration for potential environmental impacts.

The results of the development of an intelligent bivalve farmer agent to find out the best combination of bivalve seeding areas, within an allowed area of exploitation, were reported in (Cruz et al. 2007) and showed promising guidelines. One of the constraints pointed out in the conclusions of that study was the time consumed by each simulation run. Therefore the usage of a network of simulators was the natural follow up of that study.

This paper presents the specification of the network that supports the coexistence of several simulators, the adaptation of the agents' software to manage the parallel simulation of various scenarios, and the implementation of algorithms for parallel optimization, to integrate the results and decide what the best scenario is.

The next section describes the problem in analysis, followed by the presentation of the framework for ecological simulations (EcoSimNet) – its architecture and implementation. The following section refers the experiments done and the results obtained. The paper ends with an analysis of the results, the conclusions and a description of future work to be done.

PROBLEM STATEMENT

A validated ecosystem model for Sungo Bay, People's Republic of China (Duarte et al. 2003), implemented in the EcoDynamo simulator (Pereira et al. 2006) was used. The lagoon is modelled with a two-dimensional vertically integrated, coupled hydrodynamic-biogeochemical model, based on a finite difference bathymetric staggered grid with 1120 cells (32 columns x 35 lines) and a spatial resolution of 500m - Figure 1. The model has a land and an ocean boundary and the time step used was 30 seconds.

One realistic simulation for the complete bivalve culture cycle should cover approximately 1.5 years, equivalent to more than 1 576 800 simulation steps - in a computer with an Intel® CoreTM 2 CPU 6300 @ 1.86GHz and 2.00GB of RAM, the time to run the complete simulation rounds 10 hours. A previous bivalve farmer agent was developed by (Cruz et al. 2007) with the objective of finding the best combinations of locations to seed and harvest bivalve species within a delimited area of exploitation, using the previous model, towards bivalve production maximization. In that work the farmer agent had to choose the best 5 cells

(corresponding each to a 500m x 500m area) within a large region area of 88 admissible cells to explore oysters – corresponding to more than 39 millions of possible combinations. The long time and the heavy processor power required for one complete simulation, limited the previous experiments to use only 1000 simulation steps in each cycle, extrapolating the results for the complete growth cycle – the simulator runs 1000 steps in about 22 seconds and one experimental round (341 simulations) is completed in approximately 2 hours.



Figure 1 – Location of Sungo Bay, including model domain and bathimetry (Duarte et al. 2003) with delimited area of exploitation marked

The usage of a computer network allows decreasing the time needed to generate results and performing longer simulations to obtain more realistic results. The approach idealized was:

- Repeat the experiments made by (Cruz et al. 2007) using 1 and using 3 simulators, and compare the results obtained in terms of temporal savings and quality of the final solutions achieved;
- Increase the number of simulation steps and confirm if the extrapolation, regarding the results achieved, assumed previously, remains valid;
- Repeat the experiments with more cells to explore, and analyse the results.

The experiments used the algorithms implemented by (Cruz et al. 2007), controlled by a simulated annealing algorithm (Kirkpatrick et al. 1983) modified to support parallelisation and with more flexibility to control the number of simulations in each experimental round.

IMPLEMENTATION

EcoSimNet Framework

The system architecture was designed to perform complex simulations of aquatic ecosystems, to integrate easily new applications in the system, like plug-andplay hardware in computers, and enabling communications between different applications.

The Ecological Simulation Network (EcoSimNet) is based in a multi-agent architecture (Wooldridge 2002; Weiss 1999) where all the applications communicate via TCP/IP with messages formatted according to the specification of the ECOLANG language (Pereira et al. 2005). The framework can support more than one EcoDynamo simulator (Pereira et al. 2006), to allow parallel or concurrent simulations, and several agents representing the human interests over the simulated ecosystem (Figure 2).

The ECOLANG language specification forces messages to be simple, expansible, independent from any computational platform or operating system, and readable by the humans, allowing easy traceability.

This architecture permits the exploitation of machine learning algorithms with the inclusion of agents in the network (Dzeroski 2001; Russel and Norvig 2002; Pereira et al. 2004).



Figure 2 - EcoSimNet architecture

The simulator has a simple graphical user interface where users can interact with some ecological model properties – the user can select the model to use, which processes to simulate, the period of time simulated, the variables for output, and the output formats such as file or chart. Definitions such as system morphology, geometric representation, dimensions and number of model grid cells and initial values of variables and parameters are fixed when the model is created. The output files are compatible with major free and commercial software for posterior treatment, and the charts are generated through MatLab® libraries.

None of the agents have direct access to the model database. These models are available only to the simulators. The simulators provide information about the model to the agents through the ECOLANG

messages. This approach ensures true independence between the simulator and the agents.

Farmer Agent Implemented Algorithms

The base algorithm developed for the initial agent was a simple hill-climbing optimization algorithm, based on simulated annealing with Monte Carlo probability (Kirkpatrick et al. 1983; Mishra et al. 2005) - the agent seeks iteratively a new solution and saves the one with higher quality as the best. Several configurable optimizations can be activated to influence the selection logic of the new solutions (Cruz et al. 2007). The generation of the new solutions was facilitated and improved by the inclusion of known algorithms, like tabu search (Glover 1986), genetic algorithms (Holland 1975) and reinforcement learning (Sutton and Barto 1998), that can be triggered at any stage of the optimization process. The novelty of this approach is centred in the system of customizable tactics that enables the activation of any one of the implemented algorithms during the experiment, and the possibility of having, together, the various algorithms involved in choosing the best solution.

The initial agent communicates only with one simulator. To manipulate the information of several simulators, it was necessary to generate a new agent, extending the former one, and with a decision-making process that should integrate, in real time, the results from the various simulators as they were generated. The choice made was the implementation of a parallel simulated annealing algorithm (Ram et al. 1996).

Parallel Simulated Annealing Algorithm

Simulated annealing (SA) is considered a good tool for complex nonlinear optimization problems (Kirkpatrick et al. 1983) but one of its major drawbacks is its slow convergence. One way to improve its efficiency it's parallelisation (the development of a parallel version of the algorithm).

Many implementations of this algorithm exist but they are, inherently, problem dependent. (Ram et al. 1996) proposed two distributed algorithms for simulated annealing – the clustering algorithm (CA) and the genetic clustering algorithm (GCA). Both explore the evidence that a good initial solution results in a faster convergence.

The CA technique starts n nodes of the network to run SA algorithm using different initial solutions. After a fixed number of iterations, they exchange their partial results to get the best one. All the nodes accept that solution and restart the SA based on that solution. This process is repeated a predefined number of times. There must be a coordinator node to choose the best solution and to control the moment to stop and end the process.

The process implemented in our agent can be viewed as integrating the CA techniques described: the agent can accumulate the functions of coordinating (coordinator node) and generating solutions (worker node); the generation of the new solutions is driven by the tactics chosen in each agent taking advantage of their autonomy. The flexibility of the framework allows each agent to control only some simulators.

As simulators run in different computers, each one finalizes its simulation independently and the agent compares the result against all results accumulated so far; there is no need to synchronize the simulators.

The implementation carried out can work perfectly only with one agent - in this case the coordinator and the worker nodes coincide.

The basic algorithm for the coordinator node is presented in Figure 3 and the functions for the worker nodes are presented in Figure 4.

Parallel SA - coordinator node **Parameters:** initialTemperature – initial temperature temperatureModifier-decrease temperature factor N - maximum number of iterations W-number of worker agents P-number of synchronization points Global Variables: counterMS-number of missing synchronizations bestResult - best production value returned by the agents bestSolution - solution that generates the best result Algorithm: 1: for each agent w initSA (initialTemperature, temperatureModifier, N / (W * P), 0, < empty>)2: bestResult = 0; 3: bestSolution = <empty>; 4: counterMS = P; 3: while (counterMS > 0) 3.1: for each agent w runSA (); 3.2: for each agent w results[w] = collectResults (w); 3.3: choose (results[], bestResult, bestSolution); 3.4: for each agent w prepareSA (bestResult, bestSolution); 3.5: decrement (counterMS); 4: publish (bestResult, bestSolution);

Figure 3 - Parallel SA Algorithm - coordinator node

The number of synchronization points determines the number of times the worker nodes exchange partial results, and this is important to speed up the optimization process. With this process, the number of iterations is distributed uniformly by the agents (worker nodes) but not necessarily by the simulators: while the coordinator node waits for agents synchronization to exchange the partial results (Figure 3, line 3.2), each worker node controls the number of iterations with all

simulators monitored by it (Figure 4, runSA – line 3), which means that if there is one very fast simulator and other one very slow, it is expectable that the faster one runs more simulations than the slower.

Parallel SA – worker node

Parameters: temperatureModifier – decrease temperature factor NW - maximum number of iterations for worker agent Functions: neighbour(S[i]) - new solution based on S[i] neighbourhood applying agent tactics pValue(S[i]) - simulated production value for solution S[i] Global Variables: t-temperature counter-number of iterations bestResultW - best production value bestSolutionW - solution that generates the best result S[i] - solution chosen in simulator i Sn[i] -solution tested in simulator i initSA (iT, dT, nS, bR, bS) 1: t = iT; 2: temperatureModifier = dT; 3: NW = nS: 4: prepareSA (bR, bS); prepareSA (bR, bS) 1 bestResultW = bR; 2: bestSolutionW = bS; 3: for each simulator i S[i] = bestSolutionW; runSA() 1: counter=0; 2: repeat (for each simulator i) { 2.1: Sn[i] = neighbour (S[i]); 2.2: start simulation (Sn[i]); 2.3: when simulation *i* ends ł 2.3.1: result[i] = pValue(Sn[i]); 2.3.2: dS = result[i] - bestResultW; 2.3.3: if (dS > 0)2.3.4: bestResultW = result[i]; 2.3.5: bestSolutionW = Sn[i]; 2.3.6: S[i] = Sn[i];2.3.7: else if (accept Sn[i] with a probability of $min[1, e^{-dS/t}]$) 2.3.8: S[i] = Sn[i];2.3.9: t = t * temperatureModifier; 2.3.10: increment (counter); } 3 3: until (counter >= NW); 4: send (bestResultW, bestSolutionW);

Figure 4 - Parallel SA Algorithm - worker node

EXPERIMENTS AND RESULTS

Description

The new agent developed extends the previous one created by (Cruz et al. 2007) with the inclusion of the described parallel SA algorithm and a new user-friendly interface to configure and parameterize the implemented algorithms and tactics. All the experiments were done

with only one agent that accumulates the roles of the coordinator and worker nodes.

The first set of experiments tried to reproduce the experiments made by (Cruz et al. 2007) - find the best 5 cells within a large region area of 88 admissible cells to explore oysters. Each simulation runs 1000 steps (about 8 hours of real time).

The second set of experiments was performed using 3 distinct simulators; the agent communicates and configures all the simulators. The results were registered when the whole system reached 341 iterations (results collected to compare with the first set).

In the third set of experiments the number of simulation steps was increased to cover one month of oysters growth (from 1000 to 86400 steps) to verify if the extrapolation assumed in previous experiments remains valid. For this experiment 4 simulators were used.

The fourth set of experiments extended the previous one increasing the number of cells to seed to 50. Table 1 summarizes the experiments done.

 Table 1 - Experiments summary

Set	Description
1	Reproduces experiences made by (Cruz et al. 2007) with 1 agent and 1 simulator
2	Repeats set 1 using 3 distinct simulators
3	Extends set 2 to cover one month of simulation – using 4 simulators
4	Extends set 3 with more cells to seed (50)

The experiments were performed in computers with an Intel[®] CoreTM 2 Quad CPU Q9300 @ 2.50GHz, with 3.25 GB of RAM. The first set of experiments ran in about one hour and a half and the results confirm the tendencies related in (Cruz et al. 2007) – the borders are the best areas to explore: top right corner of the exploitation area is the best one (Table 2 and Figure 5).

Table 2 - Results of experimental set 1

Rank	Production Value (Tonnes)	Cells
1	169.82	71-79-85-86-87
2	169.81	39-79-85-86-87
3	169.78	70-78-84-86-87
4	169.78	52-79-85-86-87
5	169.77	31-84-85-86-87

The results showed that the inclusion of parallel SA didn't influence the results of the other algorithms. Although the results would be predictably different, the trends are comparable. In this experiment the difference

between the maximum and the minimum production value was less than 0.10% of the minimum.



Figure 5 - Visualization of the 2 best solutions (exp #1)

The second set of experiments was performed using 3 distinct simulators, and one agent that configures the simulators and accumulates the coordinator and worker roles. As expected, the time needed to achieve 341 iterations was approximately one third (35 minutes) of the initial time and the results (Table 3 and Figure 6) followed the tendency observed previously. In this experiment the difference between the maximum and the minimum production value was 0.16% of the minimum.

Table 3 – Results of experimental set	of experimental set 2
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Rank	Production Value (Tonnes)	Cells
1	169.83	71-78 -79-86-87
2	169.82	70-71-79-86-87
3	169.82	62-71-79-86-87
4	169.82	55-71-78-86-87
5	169.81	63-79-85-86-87



Figure 6 - Visualization of the 2 best solutions (exp #2)

In terms of results quality and time savings, it seems that the parallel SA is working as expected – the results maintain the tendency observed previously by Cruz et al. (2007) - and the time savings are directly related to the number of simulators in the network.

In the third set of experiments, the number of simulation steps was increased from 1000 steps to 86400 steps

(from 8h20m till about one month of real time). This experiment took about 1 day and 19 hours to finish and the results are presented in Table 4 and Figure 7. The difference between the maximum and the minimum production value was now 0.83% of the minimum.

Rank	Production Value (Tonnes)	Cells
1	7,731.80	5-28-46-50-72
2	7,725.19	19-45-60-67-82
3	7,724.11	28-50-57-61-64
4	7,722.25	27-50-59-60-66
5	7,722.06	27-53-57-58-59

Table 4 - Results of experimental set 3



Figure 7 - Visualization of the 2 best solutions (exp #3)

The results of this experiment show a spread of solutions that hardly reveals any significant trend. It is important to notice that the ecosystem in question is subjected to tides, which influence how organic substances and phytoplankton are transported along the bay. The availability of these two items – the main bivalve food sources – determines oyster growth and production.

It is no surprise that the trends revealed in the initial experiments were not confirmed, due to their very short simulation time. The simulated 8 hours is a very short period when compared to water residence time in the bay – between one and nineteen days (Duarte et al. 2003). Therefore, 8 hours is not enough to simulate properly the mixing processes and the food variability affecting oyster growth. Furthermore, when oyster biomass increases, important feedbacks to available food become apparent where local depletion of food items may limit bivalve growth (Duarte et al. 2005).

Even without an obvious tendency in the area occupation, the fourth experimental set was realized to verify if the results were more reliable when the ratio between occupied area vs. exploitation area increases – from 5,7% in the previous experiments to 56,8% in this one (seed 50 cells within the same area of 88 cells to explore). The experiment took about 1 day and 18 hours and the results are presented in Table 5 and Figure 8.

Rank	Production Value (Tonnes)	Cells
1	77,199.52	
2	77,184.49	Different
3	77,177.26	sequences of 50
4	77,137.60	cells
5	77,104.35	



Figure 8 - Visualization of the 2 best solutions (exp #4)

The solutions present different patterns but with a tendency to concentrate oysters in the upper and right sides of the exploitation area. The patterns strengthen the tendency to fill the areas near the open sea, where sea water exchanges are more intense and food tends to be more abundant.

Another important result is the coincidence in the occupied areas – the 2 best solutions share 37 cells in 50 (74%) and in the 5 best solutions more than 60% of the cells remain selected. The difference between the maximum and the minimum production value increases to 1.9% of the minimum.

CONCLUSIONS AND FUTURE WORK

This paper presented a new framework for complex ecological simulations - EcoSimNet. This framework allows the coexistence of multiple simulators in the network, controlled by different agents, enabling the simulation of different scenarios in parallel, increasing the number of simulations and the real time simulated, without compromising the quality of results and ensuring a more complete analysis of scenarios.

The results obtained showed that the time needed to reach a "near" optimal solution decreases proportionally to the number of parallel simulators in the network.

The strategy followed in the implementation of the parallel simulated annealing algorithm, separating the roles of the coordinator and the worker nodes, allowed the independence of each agent tactics for optimization; the experiments showed that the inclusion of the two roles in the same agent didn't compromise the agent's rationality. This work is a step forward towards an agent based decision support system to optimize complex environmental problems.

More experiments need to be done, increasing the number of simulators and agents in the network, in order to have a clear idea of what reasonable limits should be imposed on the size of the EcoSimNet framework.

The next steps in this platform will incorporate automatic decision in the coordinator agent, to decide how many simulators and worker agents will be necessary to consider new scenarios, and to determine degrees of similarity with scenarios already exploited. Furthermore, multi-criteria optimization simulations will be tested, where agents will evaluate different scenarios according to environmental and economical objectives.

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DISTRIBUTING REPAST SIMULATIONS USING ACTORS

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Modelling and simulation, multi-agent systems, RePast, actors, distributed simulation, HLA/RTI, Java.

ABSTRACT

RePast is a well-known agent-based toolkit for modelling and simulation of complex systems. The toolkit is normally used on a single workstation, where modelling, execution and visualization aspects are dealt with. This paper describes an approach aimed to distributing RePast models, with minimal changes, over a networked context so as to address very large and reconfigurable models whose computational needs (in space and time) can be difficult to satisfy on a single machine. Novel in the approach is an exploitation of a lean actor infrastructure implemented in Java. Actors bring to RePast agents migration, location-transparent naming, efficient communications, and a control-centric framework. Actors can be orchestrated by an in-thelarge custom control structure which can ensure the necessary message precedence constraints. Preliminary experience is being carried out using HLA/RTI as middleware. However, the realization can also work with other standard transport layers such as Java Socket and Java RMI. The paper introduces the design rationale behind mapping RePast on to actors and discusses a distributed example.

INTRODUCTION

Multi-agent systems (MAS) (Wooldridge, 2002) simulations have proved their usefulness in such diverse application domains as physics, anthropology, biology, sociology, artificial intelligence etc. However, the complexity of some MAS scalable models can be so highly demanding in computational resources to prohibit their execution on a standalone sequential computer. Therefore, the problem exists of porting a MAS on a distributed context so as to take advantage of the processing capabilities furnished by a collection of low-cost networked computers.

RePast (RePast, on-line)(Collier, on-line)(Macal & North, 2006) is a state-of-art collection of tools and libraries useful for modelling and simulation in Java of multi-agent systems. Its effectiveness has been assessed in (Tobias & Hofmann, 2004). RePast borrows much from the design of the Swarm simulation toolkit

(Swarm, on-line). A similar toolkit is SIM_AGENT (SIM_AGENT, on-line).

An experience of distributing sequential RePast over the Level Architecture/Runtime High Infrastructure (HLA/RTI) middleware (Kuhl et al., 2000) is described in a recent paper (Minson & Theodoropolous, 2008). HLA was chosen because it eases interoperability with existing simulation systems, and promotes model reuse. The implementation directly integrates the RePast mechanisms within the HLA/RTI infrastructure. A distributed RePast simulator is an HLA federation of multiple interacting instances of RePast models. Distributed synchronization depends on conservative synchronization (Fujimoto, 2000) which favours trasparency and backward compatibility with sequential RePast model. The RePast scheduling algorithm was replaced with a new one which constrains local time advancement in a federate, in synchronization with the rest of the federation. Space/environment objects are mapped on the object architecture (Federation Object Model or FOM) and the publish/subscribe pattern supported by HLA. A critical problem concerns concurrent access/update to shared attributes, e.g. of the environment. Conflicts resolution is achieved by divesting attribute ownership to RTI. All of this can have performance penalties in the runtime. A similar experimented realization was previously with distributing SIM_AGENT toolkit on top of HLA (Lees et al., 2007).

This paper proposes an original approach to distributing RePast simulations which is based on actors (Agha, 1986) and in particular on the Theatre architecture (Cicirelli et al., 2007a-b)(Cicirelli et al., 2009). Adopted actors are reactive threadless agents which communicate to one another by asynchronous messagepassing. Actors bring to RePast agents migration, location-transparent naming, efficient communications, and a control-centric framework. Actors can be orchestrated by an in-the-large custom control structure which can ensure the necessary message precedence constraints. Such standard transport layers can be used as Java Socket and Java RMI. Actors were ported also on top of the HLA/RTI middleware (Cicirelli et al., 2009) which provides, among others, transport layer and time management services. A key difference from (Minson & Theodoropolous, 2008) relates to conflict management on shared objects. In this work the recourse to attribute ownership mechanisms of RTI is avoided. Local environment and space objects are accessed in the normal way. Consistency and conflict resolution in the access to shared and remote environment variables are mediated by environment actors and messages, and harnessing features of the simulation control engine.

The achieved mapping of RePast over actors is named ACTOR_REPAST. In this paper ACTOR_REPAST design and prototype implementation is discussed in terms of preliminary experience with HLA. Other distributed scenarios are possible.

The paper is structured as follows. First RePast modelling and simulation concepts are summarized. Then the adopted actor model is presented together with a conservative distributed simulation engine. The paper goes on by discussing ACTOR_REPAST design and prototype implementation, and an adaptation of the actor-based conservative simulation engine to distributed RePast simulations. After that a model example and its execution are demonstrated. Finally, conclusions are drawn with an indication of on-going and future work

REPAST CONCEPTS

The RePast toolkit includes a runtime executive (*scheduler* and *controller* components) which furnishes an event-driven simulation engine, and a user interaction interface through which a simulation experiment can be controlled.

A system (see Fig. 1) typically consists of a collection of *agents*, a collection of *spaces* modelling the physical environment within which the agents are situated (have coordinates) and operate, and a *model* object which contains information (e.g. for configuration) about the entire system. The *state* of system is scattered among model, agent and space objects. An agent-based simulation normally proceeds in two stages. The first one is a setup stage that prepares the simulation for execution. The second stage is the actual running of the simulation. During the setup phase, the model object is created as an instance of a Model class



Figure 1: Starup scenario





(implementing the SimModel interface) which makes instances of agents and spaces, display and scheduler (the latter is an instance of the Schedule class). It is the executive which actually asks the model object to execute the setup phase. After that, when the simulation is started, the executive achieves from the model object the scheduler object used to control the simulation. Fig. 1 summarizes the operations of model bootstrap, whereas Fig. 2 depicts model execution.

RePast events are instances of the BasicAction class. An event occurrence is mirrored by an invocation of the execute() method of a basic action object. Actions are scheduled to occur at certain simulation times (ticks). Ticks can be equally spaced or, more in general, not equally-spaced or event-driven. All pending events existing at a given moment are buffered, ranked by ascending timestamps, within the scheduler object. At each iteration of its control loop, the controller asks scheduler to extract the (or one) most imminent pending action and to dispatch it to its destination object, i.e. model or agent. The consequence of an event occurrence is in general a chain of method invocations, which can cause state changes in agents, in model or in space objects.

Space objects can be *data* (or *diffusive*) *spaces* or *object* (*agent*) *spaces*. An application based on diffusive spaces typically has the model which repeatedly executes a cycle made up of three basic phases: *diffuse- modify-update*. During the diffuse phase, the environment is asked to synchronously update itself according to a diffusive logic. Then, in the modify phase agents are allowed to introduce further changes to the data space. For consistency, though, these changes are stored in a temporary copy of the environment. Finally, in the update phase, the temporary copy is restored on the actual environment. An object space, on the other hand, behaves more asynchronously. Agents can issue get/put operations to

spaces, which affect immediately the environment. At each tick, the Model object causes the environment changes to be displayed by invoking the Display *redraw* method.

ACTORS

The following gives an overview of a variant of the Actor model (Agha, 1986) which is used for distributing RePast. The same architecture is being experimented for supporting Parallel DEVS (Zeigler et al., 2000)(Cicirelli et al., 2008). Actors (Cicirelli et al., 2009) are reactive thread-less objects which encapsulate a data state and communicate to one another by asynchronous message passing. Messages are typed objects. Actors are at rest until a message arrives. Message processing is atomic: it cannot be suspended nor preempted. Message processing represents the unit of scheduling and dispatching for a theatre. The dynamic behavior of an actor is modeled as a finite state machine which is realized in the handler(message) method which receives the message to process as a parameter. Responding to a message consists in general of the following actions:

- new actors are (possibly) created
- some messages are sent to known actors (*acquaintances*). For proactive behavior, an actor can send to itself one or more messages
- the actor migrates to another execution locus (theatre, see below)
- current state of the actor is changed (become operation).

Actor mechanisms are supported in Java by a minimal API. Actor classes derive directly or indirectly from the Actor base class. Similarly, message classes derive from the Message base class. A subsystem of actors allocated for execution on a computing node of a networked context is treated as a unit-in-the-large and is termed a *theatre*. A theatre furnishes the communication (including migration), scheduling and dispatching message-based services to actors. A fundamental component of a theatre is the *control machine* which interacts with peers in a distributed context through a suitable transport layer.

A migrating actor leaves on the originating theatre a *forwarder* (proxy) version of itself which will route incoming messages to the destination theatre where the real version of the actor exists. To avoid multi-hop communications, the address information of a moving actor is updated on the source theatre so as to mirror current actor location.

CONSERVATIVE CONTROL ENGINE

Control machines of a distributed system are required to coordinate each other according to a specific control structure in order to guarantee messages are ultimately executed in timestamp *and* causal order during a distributed simulation (Fujimoto, 2000). The actor model was implemented in a case on top of IEEE 1516 standard HLA/RTI middleware (Cicirelli *et al.*, 2008)(Kuhl *et al.*, 2000)(Pitch, on-line) whose in-built time management services can be exploited to achieve, e.g., a conservative distributed simulation engine like the one outlined in the following.

A theatre naturally maps on to an HLA federate. It is assumed that the theatres/federates of an HLA federation are both time constrained and time regulating. Each theatre asks RTI for a time advancement through Next-Event-Request-Available (NERA) calls (zero lookahead) (Kuhl et al., 2000). Simulation (or virtual) time grows according to model time. However, at a given model time, simultaneous or contemporary events are handled by a tie-breaking mechanism which ranks events on the basis of their generation. The generation concept is useful to ensure cause-effect relationships among messages. Of course, the effect has always to be processed after its cause. For example, contemporary messages created by an actor in the course of responding to an incoming message m, can be managed in the next generation with respect to the generation of m. The logical time presented to HLA/RTI through a NERA is actually a triple <virtual-time, generation, step>. virtual-time is the model time. The (optional) step field acts as a least significant bit of generation. The control structure can use the step field to further discriminate some concurrent messages. For instance, a migration request can purposely be delayed at the end of current generation to ensure pending messages destined to the migrating actor are processed in the source theatre before migration. All of this can be achieved by scheduling the migration to occur at step=1 of current generation, and waiting from RTI the corresponding release of Time-Advance-Grant.

A specialization of the above control strategy was implemented to support Parallel DEVS models (Cicirelli *et al.*, 2008). Another adaptation is discussed later in this paper as part of distributing RePast.

ACTOR_REPAST

A RePast model is partitioned into a collection of Logical Processes (LPs) which are allocated for the execution on different computing nodes of a networked system. The structure of nodes/LPs is summarized in Fig. 3. Each LP hosts a portion (*region*) of the environment and a subset of agents (mapped as actors). Agents can migrate from an LP to another at runtime. The following points out basic problems arising from partitioning and the particular software engineering solutions which were adopted to cope with them. Mapping issues essentially fall in three main areas: state space representation, scheduling system, conflict resolution on shared variables.

Partitioning and Region Boundaries

Partitioning mainly splits environmental spaces into regions assigned to distinct LPs. As suggested by Fig. 3, the RePast model is "instantiated" on *each* participating


Figure 3: Architecture of a networked RePast model

Mapping Design Rationale

node. In reality, only the environment portion relevant to each particular node gets effectively instantiated at configuration time. Configuration will assign real or proxy versions of the agents (actors) to the various nodes which comprise the distributed system. Of course, the display facilities into each node are relative to the environment portion managed by the node. As a consequence of instantiating the "entire" model on every node, the Model object gets replicated on each node. However, only the Model object in the master node (designated at configuration time) is allowed to start-up the simulation by scheduling the initial actions. In the following it is assumed that a RePast agent perceives only a part of its environment identifiable as its neighbourhood (or "sphere of influence" (Logan & Theodoropoulos, 2001)). Environmental region boundaries introduce shared variables for the agents belonging to adjacent LPs. A detailed look at region boundaries is exposed in Figures 4 and 5 where the border of two neighbouring LPs is shown. More complex boundary scenarios can occur in practice. In particular, Fig. 5) clarifies that the border region of an LP is in reality composed of two parts: a local border of the LP and a mirror border of the local border of the adjacent LP. The mirror parts are replicas of boundary space cells. A first problem raised by boundary regions is the requirement of keeping consistent local and mirrored parts. An update to a boundary local cell must be reflected also in the mirror part. A second problem concerns conflict resolution during concurrent accesses to shared space cells by agents executing in the two LPs. In the approach described in this paper, conflicts are resolved by harnessing mechanisms of the distributed simulation engine (see later in this paper).



Figure 4: Boundary regions of two adjacent LPs

Mapping design was guided by the goal of maintaining a distributed model almost transparent with respect to the sequential model. In the proposed mapping, local action executions behave exactly as in the non distributed version of the RePast model. However, remote action requests, i.e. when the target agent is located on a remote LP, are captured in actor messages and sent across the network. To achieve this effect, agents and model object of a RePast system are turned into actors. Since agents have no special constraints in RePast, a (minimal) requirement was added to develop agent classes and model classes respectively as heir of base classes ACTOR AGENT and ACTOR MODEL, which derive from Actor and provide relevant common behaviour. Action objects are transformed into messages and scheduled in the theatre's control machine of the LP. A key point of ACTOR_REPAST is a transfer of control responsibilities from RePast to theatre control machine. Basically, RePast controller remains in charge of interactive events only. Simulation and time management services are instead provided by theatre control machines.

To figure out common behaviour of actor-agents, the handler(incoming_message) method of ACTOR_AGENT is actually responsible of invoking a specific method (whose name is stored in the incoming message) of the corresponding RePast agent, with the help of Java reflection. As another example, when a message is up to be dispatched to a forwarder, i.e. a



Figure 5: Detailed view of border regions

proxy of a moved actor, the behaviour in ACTOR_AGENT manages to route the message to the corresponding remote actor. Similar behaviour is provided by ACTOR_MODEL. It is worth noting that a model object does not require migration.

A more general task is accomplished by *interceptors*, i.e. entities which intercept method calls and superimpose to them suitable behaviour, with the goal of minimizing "code intrusion" in the original RePast model. Interceptors are realized as *cross-cutting concerns* or *aspects* (Kiczales *et al.*, 2001) of AspectJ (AspectJ, on-line).

An aspect controls the execution of the chain of method calls triggered by dispatching an action. When the target agent of a method invocation is local, the aspect lets the agent to execute the method call in the normal way. In the case the receiver is remote, the aspect replaces the standard behaviour of method call by building a message, filling it with information about the requested method, and sending the message over the network. A second aspect is concerned specifically with capturing action scheduling requests in the RePast model and redirecting them to the theatre control machine. A third aspect is used during the start-up phase of a model to inhibit initial action scheduling in non master LPs. Therefore, the Model object really executes only in the master LP.

An important actor in every LP, created at start-up time, is the "environment actor" (EnvActor) which knows about configuration information (taken from a configuration file) of the entire RePast model, and offers a common interface to the model for accessing spaces and environments. For example, the idea that every node/LP is an instantiation of the "entire" model implies that into each sub-model assigned to an LP be present the "global view" to the environment. The transformation of positional coordinates for a situated agent from the global-view to the local-view corresponding to the portion of the environment effectively managed by the LP is accomplished by the EnvActor. A second responsibility of EnvActor is that of propagating to its peer(s) in neighbouring LP(s) the updates of agents in the local border of the belonging LP. Similarly, when an agent moves to the border region, the EnvActor is in charge to migrate the agent, if required, to a neighbour LP. EnvActor is also a key for the diffuse/update/redraw processes. In particular, when the model in the master node raises а diffuse/update/redraw operation, the request is intercepted and a corresponding message is created and sent to all the LPs, which is heard by the EnvActors. An EnvActor then acts so as to actuate the diffuse/update/redraw operation in the local environment.

Distributed Simulation Engine and Conflict Management

An HLA distributed RePast model is governed by an adaptation of the conservative simulation engine

previously reported in this paper. The adaptation concerns a particular use of both the generation and step fields of the time notion presented to RTI, with the goal of controlling contemporary messages occurring at a given simulation time. More precisely, the generation field is used to resolve conflicts on shared environment border objects by constraining adjacent LPs to make requests to conflicting objects at *different* real times. All of this is achieved by assigning to conflicting agents a different occurrence generation. The step field, instead, is devoted, at each generation of current time or to next simulation time, to ensure that update operations to border cells are definitely propagated to adjacent LPs before such updates are visible to the model. Toward this, all updates to border cells are captured by an EnvActor and collected into a bag message, one for each distinct adjacent LP. Each bag message is sent across the network to be processed at step=1 of current generation. Therefore, when bags are eventually received and processed by corresponding EnvActors, their effect will only be heard at the next generation or next tick. Also at step=1 are realized agent migrations.

At the beginning of any simulation time, a method of the EnvAct is launched which analyzes the border area and assigns to potentially conflicting agents different generation numbers. These numbers are stored and will be used for scheduling, at current simulation time, action messages or method invocation messages triggered by an action, directed to border agents. It is worth noting that agent population of the border regions of two adjacent LPs is identical. Moreover, the algorithm is run at both sides of the adjacent LPs and makes an identical assignment to the same agents of the border area. In the following, the operation of the algorithm will be sketched in the hypothesis of having agents which can move to a next position with unit distance. Fig. 6) shows an example of border (potentially) conflicting agents. Recall that a border region (see also Figg. 4 and 5) is composed of two sub regions, one corresponding to a local area of the LP, the other to a mirror of the local area of adjacent LP. In addition, in the hypothesis of unit-step movements, the two sub-regions are concretely two columns wide. Fig. 7) depicts a worst case situation of conflicts where 7



Figure 6: Example of (potentially) conflicting agents



Figure 7: A worst case conflict situation

generation numbers are sufficient for resolving conflicts.

The algorithm proceeds by scanning the complete border area of the LP starting from the upper left corner down to (in row order) the right corner in last row. For each agent (denoted ? in Fig 7)), its relevant neighbourhood is examined. For the agent ? in Fig. 7) the relevant neighbourhood is represented by the dashed rectangle. In fact, the lower part of the neighbourhood is still not assigned, and the upper right part is composed of agents belonging to the same adjacent LP. In the worst case scenario all previously assigned agents in the relevant neighbourhood have received distinct generation numbers. Generations of assigned agents in the relevant neighbourhood are marked as unavailable for the current agent. Then a generation, randomly chosen in the set of available generations, is assigned to current agent. The algorithm naturally reuses generations and this is important both to keep low the number of exploited generations but also to increase the concurrency degree of border agents. Determinacy of the algorithm (at both sides of adjacent LPs) relies on a pseudo-random generator whose seed, at each choice, is defined in terms of current simulation time and the agent environmental position. Moreover, determinacy is also ensured by the scanning order of the border area.

It should be noted that border agents without conflicts are always assigned the first generation (numbered 0) of a simulation time. In addition, both local agents and border local agents without conflicts are handled exactly in the same way.

An Example

ACTOR_REPAST was preliminary tested by using some sequential models available in the software distribution of RePast version 3. The following demonstrates ACTOR_REPAST operation by distributing the Swarm-based HeatBug multi-agent model, which is representative of a class of models



Figure 8: A screenshot from sequential RePast simulation of the HeatBug model

where the environment component admits both diffusive and agent object spaces. The system model logically consists of two parallel grids: the first one is populated by heat bug agents. The other grid is employed for diffusing from cell to cell the heat owned by bugs. The diffusion logic is already available in the implementation of RePast diffusive spaces. Heat bugs are simple agents which absorb and expel heat. Heat bugs have an ideal temperature and will move in an attempt to achieve this temperature.

Fig. 8 shows a screenshot taken from RePast sequential model execution. As one can see, bugs tends definitely to group so as to reach their ideal temperature.

For demonstration purposes, the sequential HeatBug model was partitioned into two LPs and executed, under ACTOR_REPAST, on two theatres/federates on top of HLA pRTI 1516 (Pitch, on-line). The two federate are allocated to two distinct physical processors consisting of WinXP platforms, Pentium IV 3.4GHz, 1GB RAM,



Figure 9: A screenshot of the two display taken from ACTOR_REPAST

interconnected by a 1Gb Ethernet switch. The distributed system naturally exhibits agent migration from an LP to the other. The system was configured (in an XML configuration file, one per LP) with such information as: (a) the list of LPs, each one specified by <IP address, port>, (b) the master LP identification, (c) the topology of the distributed model, with definition of LP adjacency and size of the border regions. Fig. 9 shows the display produced by the two LPs, which confirm the basic behaviour of the bug agents.

Other architectural scenarios are possible specifically for the visualization purposes. For example, as in (Low *et al.*, 2007) one single federate (time constrained but not time regulating) could be dedicated only to visualization.

Conclusions

This paper describes an approach and prototype implementation to distributing RePast (Collier, on-line) simulations. The realization, ACTOR_REPAST, owes to a lean and lightweight actor framework in Java which allows customization of the simulation control engine. Preliminary experiments are being carried out using the HLA/RTI 1516 IEEE standard (Kuhl *et al.*, 2000)(Pitch, on-line). Other distributed and transport layers, though, are possible.

Prosecution work is geared at:

- improving the transformation from sequential RePast models to corresponding distributed versions through a systematic exploitation of Java *text annotations* which would help tagging source classes and methods and hiding behind annotation management the necessary yet transparent code changes
- optimizing the algorithm which assigns generations to conflicting agents on border regions. More in general, a fundamental open issue concerns the evaluation of different organizations of the environment component of multi-agent systems (Logan & Theodoropoulos, 2001)
- using ACTOR_REPAST in very complex agentbased models with the goal of quantifying specifically the simulation performance towards a comparison with the implementation described in (Minson & Theodoropoulos, 2008).

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SimAgent,

STATECHART-BASED ACTORS FOR MODELLING AND DISTRIBUTED SIMULATION OF COMPLEX MULTI-AGENT SYSTEMS

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Multi-agent systems, statecharts, modelling and simulation, distributed simulation.

ABSTRACT

This paper discusses the use of Theatre, a multi-agent simulation architecture, for the distributed simulation of discrete event systems (DESs) whose entities express complex behaviours. Complexity is dealt with by exploiting statechart-based actors which constitute the basic building blocks of a model. Actors are lightweight reactive autonomous agents that communicate to one another by asynchronous message passing. The threadless character of actors saves memory space and fosters efficient execution. The behaviour of actors is specified through "distilled statecharts" that enable hierarchical and modular specifications. Distributed simulation is accomplished by partitioning the system model among a set of logical processes (theatres). Timing management and intertheatre communications rest on High Level Architecture (HLA) services. The paper highlights the current implementation status and demonstrates the practical application of the approach through a manufacturing system model.

INTRODUCTION

The size and the complexity of systems which are usually modelled as discrete event systems (DESs) (e.g. communication networks, biological systems, weather forecasting, etc.) is ever increasing. Modelling and simulation of such systems is challenging in that it requires suitable specification languages and efficient simulation tools.

Multi-agent architectures (Wooldridge, 2002) have proven to be effective in exploiting parallel and distributed computing environments for the simulation of DESs involving a large number of interacting entities (Cicirelli *et al.*, 2009)(Cicirelli *et al.*, 2007) (Jang *et al.*, 2003). In this context, state-based formalism have been successfully used for specifying agent behaviours. However, as each single agent may express a complex behaviour such languages have to face the well-known state-explosion phenomenon which is typically addressed by resorting to hierarchical and modular constructs.

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) Statecharts (Harel, 1987)(Booch *et al.*, 2000) are an extension of classical state transition diagrams which have such type of features. The basic mechanism consists in the possibility of nesting a sub automaton within a (macro) state thus encouraging step-wise refinement of complex behaviour. In addition, a macro state can be *and*-decomposed for supporting a notion of concurrent sub automata. Statecharts have been successfully applied to the design of reactive event-driven real-time systems (Harel & Polity, 1998)(Selic & Rumbaugh, 1998)(Furfaro *et al.*, 2006), as well as to modelling and performance analysis, e.g. (Vijaykumar *et al.*, 2002-2006).

This paper discusses the use of a Java framework which supports the execution of agents whose behaviour is modelled by means of statecharts. The approach improves previous authors' work (Cicirelli et al., 2008) by extending it to the context of a distributed-simulation architecture named Theatre (Cicirelli et al., 2009). A particular notion of agents is adopted which rests on actors (Agha, 1986). Actors are lightweight, threadless reactive components which communicate to one another by asynchronous message passing. An actor is characterized by its message interface, a set of hidden data variables and a behaviour for responding to messages (events). A multi-actor subsystem (theatre) is orchestrated by a control machine which provides basic timing, scheduling and dispatching message services to actors. In this paper the behaviour of an actor is specified through a "distilled" statechart, where only the or-decomposition of states is admitted. Concurrent sub states are avoided. The approach is demonstrated by applying statechart actors to modelling and simulation of a manufacturing system. Results from simulation experiments are reported. Finally, conclusions are presented together with indications of future work

THEATRE

The architecture of Theatre consists of two main parts:

Execution platforms, i.e. theatres, which provide 'in-the large' features, i.e. the environmental services supporting actor execution, migration and interactions. Services are made available to actors through suitable Application Programming Interface (APIs). • Actor components, i.e. the basic building blocks 'in the-small', which capture the application logic. While Theatre can be hosted by different object-

oriented programming languages, the implementation considered in this work refers to Java.

Actor modelling with Statecharts

Actors are reactive objects which encapsulate a data state and communicate to one another by asynchronous message passing. Messages are typed objects. Actors are at rest until a message arrives. Message processing is atomic: it cannot be suspended nor preempted. Message processing represents the unit of scheduling and dispatching for a theatre. The dynamic behavior of an actor is specified by means of a state machine, which, in the context of this work, is a statechart-based hierarchical state machine.

A state of a hierarchical state machine can recursively be decomposed into a set of sub states, in which case it is said to be a *macro* state. A state that is not decomposed is said to be a *leaf* state. The root state of the decomposition tree is the only one having no parent and it is referred to as the *top* state.

Statecharts admit two types of state decomposition: ordecomposition and and decomposition (Harel and Politi, 1998). In the former case a state is split into a set of sub states which are in an "exclusive-or" relation, i.e. if at a given time the state machine is in a macro state it is also in exactly one of its sub states. In the latter case sub states are related by logical "and", i.e. if the state machine is in a macro state it is also in *all* of its direct sub states, each of which acts as an independent concurrent component. The type of statecharts used for modeling actor behavior are "distilled", in the sense that they permit only the ordecomposition and thus the single actor is the unit-ofconcurrency. All of this complies with the basic assumptions of the adopted actor computational model where concurrency exists at the actor level but not within actors. In other words, concurrency stems from reacting to messages and not from the use of heavyweight multi-threaded agents which can have space/time constraints in the M&S of large systems. A message reaction represents an atomic action which can modify the actor internal data, generate messages to known actors (acquaintances) including itself for pro-activity, create new actors, change the current state of the actor.

At a given point in time, an actor finds itself simultaneously in a set of states that constitutes a path leading from one of the leaf states to the top state. Such a set of states is called a *configuration* (Harel and Naamad, 1996). A configuration is uniquely characterized by the only leaf state which it contains.

Each macro state S specifies which of its sub states must be considered its *initial state*. This sub state is indicated by means of a curve originating from a small solid circle and ending on its border. This curve, although technically is not a transition, is referred to as the *default transition* of S. State transitions are represented by edges with arrows. Each transition is labelled by *ev[guard]/action* where *ev* is the trigger (event causing the transition), *guard* a logical condition which enables the transition when it evaluates to true, and *action* the action "à la Mealy" associated with the transition.

Both source and destination of a transition can be states at any level of the hierarchy. Whereas a transition always originates from the border of a state, it can reach its destination state either on its border or ending on a particular element called *history connector* or *H*connector. Such a connector is depicted as a small circle containing an *H* (*shallow history*) or an H^* (*deep history*), and it is always inside the boundary of a compound state.Firing a transition leads the actor to switch from one configuration to another. When a configuration is left, each of its macro states keeps memory of its direct sub state that is also part of the configuration. This sub state is referred to as the *history* of the macro state. The first time a state is entered, its history coincides with its initial state.

Let S be the destination state of a transition tr. The configuration which is assumed as consequence of firing tr depends on the way tr reaches S:

- If *S* is a leaf state the new configuration is the only one that contains *S*.
- If *S* is a macro state and *tr* ends on its border, the next configuration corresponds to the destination state being the initial state of *S*.
- If *S* is a macro state and *tr* ends on a shallow history connector, the next configuration corresponds to the destination state being the state that is the history of *S*.
- Finally, if *S* is a macro state and *tr* ends on a deep history connector, the configuration depends on the nature of the state *D* which is currently history of *S*. If *D* is a leaf state, the configuration will be the only one that contains *D*, otherwise the configuration corresponds to the case *tr* would end on a deep history connector of *D*.

Each state can have entry/exit actions which are respectively executed each time the state is entered or exited. Moreover, within a state can be present "internal transitions" which denote incoming events which are processed *without* leaving/re-entering the state. Therefore, an internal transition never triggers exit/entry actions into execution. The concept differs from self-loop transitions which imply execution of exit/entry actions of the state.

Theatre architecture

Fig. 1 depicts the architecture of Theatre. Each theatre node has the following components:

- an instance of the Java Virtual Machine (JVM)
- a Control Machine (CM)
- a Transport Layer (TL)
- a Local Actor Table (LAT) and
- a Network Class Loader (NCL).

The Control Machine hosts the runtime executive of the theatre, i.e. it offers basic services of message scheduling/dispatching which regulate local actors. The Control Machine can be made time-sensitive by managing a time notion ("real" or simulated). Actually, the Control Machine organizes all pending (i.e. scheduled) messages in one or multiple message queues. Instead of having one mail queue per actor (Agha, 1986), the Control Machine buffers all sent messages and superimposes them an applicationdependent control strategy.

During the basic control loop, a pending message is selected (e.g. the (or one) most imminent in time) and dispatched to its destination actor to whom is given the possibility of executing a relevant state transition. After the transition code is executed, the control loop is reentered, all messages sent by the last activated agent are scheduled and, finally, the next cycle is started.

The Transport Layer furnishes the services for sending/receiving network messages and migrating agents. Details about the lightweight migration mechanism are described in (Cicirelli *et al.*, 2009).

As an example, Java Sockets or Java Remote Method Invocation (RMI), based on reliable Transmission Control Protocol (TCP) FIFO channels, can be used as a concretization of the Transport Layer. They are part of existing implementations of Theatre.

The Local Actor Table contains references to local agents of the theatre. The Network Class Loader is responsible for getting dynamically and automatically the class of an object (e.g. a migrated agent) by retrieving it from a network Code Server acting as a code repository for the distributed application.

Control machines in a Theatre system have to coordinate each other in order to ensure a global synchronization global strategy. Different synchronization algorithms were implemented on top of Theatre. In (Cicirelli et al., 2007) a time warp based simulation control engine (Fujimoto, 2000) is described which uses state-saving and rollback mechanisms to implement an optimistic distributed simulation framework. In (Cicirelli et al., 2009) a conservative synchronization structure (Fujimoto, 2000) is proposed which is based on HLA and is capable of handling actor migrations. A specialization of this global control strategy with a tie-breaking mechanism for managing contemporary or simultaneous messages, i.e. occurring a same simulation time, and required to fulfil precedence constraint relationships, is described in (Cicirelli et al., 2008) for supporting specifically the execution of Parallel DEVS (Zeigler et al., 2000) systems realized over theatres and actors. In this paper, the conservative simulation algorithm proposed in (Cicirelli et al., 2009) is assumed for the distributed simulation experiments based on statechart actors.



Figure 1: Theatre architecture

A MODELLING EXAMPLE

This section illustrates an application of the approach by considering a model of a manufacturing system. The example is adapted from (Vijaykumar *et al.*, 2002-2006) where it has been handled by statecharts with *and*-decomposition and event broadcasting (Harel & Politi, 1998), and analytically studied by preliminarily transforming the model into a continuous time Markov chain (CTMC). In this paper the model is simulated. Obviously, simulation opens to the possibility of using probability distribution functions for event occurrences beyond the exponential one which is normally a prerequisite for building a CTMC. In addition, simulation can be exploited for investigation of more general properties about system behaviour.

In the considered manufacturing systems (Fig. 2), two machines, respectively referred as Machine A and Machine B, operate in series processing the submitted jobs for producing a single product. Jobs are first processed by Machine A and then by Machine B. A bounded capacity Inventory is used for decoupling the operation of the machines thus reducing their wait times. A Robot is actually in charge of loading/unloading the two machines with jobs, possibly using the Inventory for temporary job buffering. Both machines and the robot may be subject to failures. Repairing from a failure is responsibility of an Operator.

Machines, Robot, Operator and the Inventory are modelled as actors. Event broadcasting, which was present in the original model, is replaced by direct communications. In particular, because the robot bases its decisions on the operation state of the two machines and of the inventory, it gets directly notified by these components about relevant state changes. Analogously, when the robot, or one of the machines, goes in a failure state it directly asks the operator for being fixed.

Statechart Models

Figures from 3 to 6 depict the statecharts modelling respectively the behaviours of Machine, Operator, Inventory and Robot actors. The top states of all these statecharts have a default state named New, which is a leaf state, where each actor waits for the arrival of an Init message carrying initialization information. After being initialized, a machine (see Fig. 3) goes into state W where it waits for a job to be processed.



Figure 2: A manufacturing system model



Figure 3: Machine behaviour

From W, it moves into state P when it has been loaded by the robot with a job. While residing in state P the machine processes the loaded job. At processing end, the machine moves into WU waiting for being unloaded. Both states W and WU have an entry action that consists in sending a Notify message to the robot for letting it know that the sending machine needs to be loaded or unloaded.

The message EndProcess is an internal message which a machine sends to itself for simulating the processing time (dwell time in P). During its stay in P, a machine can be subject to a failure in which case it moves to state B. As for processing end, failure is also modelled by another internal message which the machine sends to itself according to the next time to failure defined by a corresponding probability distribution function. When a Failure message is received, a request for being fixed is sent to the operator through a Repair message. After being repaired (arrival of the external message EndRepair coming from the Operator), the machine can return into state P for continuing processing of the interrupted job, or it can go back to W in the case the partial processed job is lost. The two possibilities are controlled by the boolean variable loss whose value is determined accordingly to the specified loss probability.

The behaviour of the Operator is depicted in Fig. 4. After being initialized, it waits in state W for a repairing request. As soon as such a request is received it moves into state R. The Operator resides in R for a dwell time that models the repairing time whose mean duration changes depending on the actor (a machine or the robot) that has made the request. While in R, other repair requests may arrive. They are handled by an internal transition whose action consists in storing them into suitable internal variables, thus postponing their processing. The completion of the repairing process is achieved with an internal message EndProcess to which the actor reacts by sending an EndRepair message to the relevant actor and a Check message to itself. Upon receiving a Check message, the operator inspects its internal variables for checking whether there are pending repair requests. When faced with the decision of which entity to repair first, the operator chooses according to the following priority order: first machine Mb, then machine Ma and lastly the Robot.



Figure 4: Operator behaviour



Figure 5: Inventory behaviour

The behaviour of the Inventory is portrayed in Fig. 5. It is a bounded buffer of capacity n, which can be 0 or a positive value. After initialization, the Inventory can be in one of the states among Empty, Partial or Full. Depending on the current available space, a Get/Put message can switch the inventory between Empty, Partial or Full as shown in Fig. 5. All of these three states have an entry action which consists in notifying the robot about the current inventory state.

The robot is the most complex entity as can be seen from the statechart of Fig. 6 which models its behaviour. While in state W, the robot waits for an operation to be exercised on the machines. Whenever the robot receives a Notify message it always updates its internal variables according to the received information. This is mirrored by the internal transitions of states W, P and B. In particular, if the robot gets notified when it is in state W, it proactively sends to itself a Check message. On the basis of the information about the state of the other components, if it is able to do some operation when the Check message is received, it switches to macro state P and sends to itself a Start message.



Figure 6: Robot behaviour

This condition is reflected by the value of the boolean variable condP which is the logical or of various conditions as summarized in Table 1.

State D is the default sub state of P which is left as soon as the Start message is delivered. At least one of the guards of the transitions leaving D is satisfied because each of them implies condP (see Table 1). The robot gives priority to unloading machine Mb (cond1 and sub state U2), then to simultaneously unloading machine Ma and loading machine Mb (cond2 and sub state UL), then to loading machine Mb (cond3 and sub state L2), then to unloading machine Ma (cond4 and sub state U1) and, finally, to loading machine Ma (cond5 and sub state L1).

The time spent by the robot in any operating state depends on the particular operation (see Table 2) that it is accomplishing. The internal message End is self-sent for witnessing the end of the operation, in which case the robot moves first into the E state and then sends itself a Passivate message whose arrival takes the robot from state P to state W where the behaviour repeats again.

The transition having Failure as the trigger message is an example of a group transition. It means that whatever is the internal sub state of P, the arrival of the Failure message causes the state P to be exited and state B to be entered, where the Robot requires to be repaired by the Operator.

Table 1: Environmental conditions for the robot			
cond1 = Mb is in WU;			
cond2 = Ma is in WU && Mb is in W;			
cond3 = Mb is W &&(Inv is empty);			
cond4 = Ma is in WU && –(Inv is Full);			
cond5 = Ma is in W;			
condP = cond1 cond2 cond3 cond4 cond5;			

Table	2:	Simulation	p	arameters

	Machine A	Machine B	Robot
Production rate	β _A =8,10 or 12	β _B =10	
Failure rate	λ _Α =1	λ _B =0.5	λ =1
Repairing rate	μ _A =10	μ _B =15	μ ε=10
Loss probability	p _A =0.5	рв=0.3	
Loading rate			γ _{L1} =100
machine A			
Unloading rate			δu1 =100
machine A			
Loading rate			γ _{L2} =100
machine B			
Unloading rate			δ _{U2} =100
machine B			
Moving rate from			α _{UL} =70
m. A to m. B			

While the Robot is in an operating state, it can fail (internal message Failure received). In this case the ongoing operation is interrupted and the operator is asked for intervention. Which event arrives first between End and Failure depends on the next time respectively for completing the operation and for failing.

The transition triggered by EndRepair causes the Robot to return into macro state P with history (see the shallow connector history H). This way, the actor returns exactly into the internal sub state of P which was current when P was last left off at the time of Failure.

For the purpose of experimentation, all the timed events in the system are assumed to be exponentially distributed. Table 2 summarizes the rates (number of events per time unit) used for simulation (as in (Vijaykumar et al., 2002-2006)). Loading/unloading rate of machines are shown as dwell times in the corresponding operation state of the robot.

Simulation results

The manufacturing model was simulated using the parameter values in Table 2, with the aim of validating the distributed runtime infrastructure of statechartbased actors. Simulation uses dense time. Each experiment lasts after a time limit of $tEnd=5\times10^5$. The model was split in two Logical Processes (LPs)/federates assigned to two distinct processors (Pentium IV 3.4GHz, 1GB RAM) interconnected by a 1Gb Ethernet switch in the presence of HLA (pRTI 1516). One LP was assigned the machines and the Operator, the other LP the Robot and the Inventory. Into each LP is also present a Monitor actor for collecting useful information about the simulation. Each monitor has methods for capturing such data about system productivity, utilization of machines, robot and operator, losses in machines, average inventory size etc. In addition, every monitor sends to itself, at the beginning of the simulation, a timed message to be received at tEnd. Following the arrival of such a message, the actor displays collected statistical information.

The system model was studied in three cases: when machine A has respectively a lower/equal/greater production rate than B (see Table 2). System properties were analyzed vs. the inventory bounded capacity which was varied from 0 to 20. Experimental results comply with those reported in (Vijaykumar *et al.*, 2002-2006), but furnish more detailed information about system behaviour.

Fig. 7 portrays measured system productivity (number of unloads from machine B per time unit) vs. the inventory capacity. As one can see, starting from 0, an increase in the inventory capacity increases the system productivity until the system reaches full-busy condition. In this condition the system exhibits maximum parallelism among components, with the inventory which smooths out instantaneous differences in the production speed of the two machines. The smoothing effect is obviously greater when the production rate of machine A grows.

The positive effect of using a not zero inventory size can be checked in Fig. 8 which shows the waiting time for unloading machine A vs. the inventory capacity. This statistic was achieved by summing up the dwell time of machine A in state WU, waiting for the robot to unload the finished product, and then dividing the sum for the simulation time limit.

For completeness, Fig. 9 illustrates the wait time for unloading machine B, which has priority with respect to unloading machine A. As expected, machine B has a small wait time.

CONCLUSIONS

This paper describes and demonstrates, through an example, an approach to modelling and distributed simulation of multi-agent systems. Novel in the proposed approach is an exploitation of a lightweight actor computational model which permits the behaviour of each agent to be specified through a "distilled" statechart (Harel, 1987). All of this favours the expression of complex behaviour at the agent level. Complexity in the large is dealt with by the Theatre architecture (Cicirelli *et al.*, 2009) which allows decomposition of a large system into sub-systems (theatres) each hosting a collection of application actors, allocated for execution on a physical processor. Actors are capable of migrating from a theatre to another, e.g. to cope with demands of dynamically

reconfigurable systems (Cicirelli *et al.*, 2009) or to respond to load-balancing requirements.



Figure 7: Observed system productivity vs. inventory capacity.



Figure 8: Average wait time for unloading machine A



Figure 9: Average wait time for unloading machine B

Theatre and statechart actors, in a case, were implemented on top of HLA services (Kuhl *et al.*, 2000)(Pitch, on-line) in the presence of conservative synchronization.

On-going and future work are geared to:

- modelling and simulation of large, scalable and reconfigurable systems in order to study the execution performance issues;
- extending the approach with optimistic synchronization, e.g. by implementing a Time Warp based distributed simulation algorithm (Fujimoto, 2000)(Cicirelli *et al.*, 2007b);
- improving M&S capabilities by experimenting with environment-based multi-agent systems (Logan & Theodoropoulos, 2001).

The last point deserves some further comments. The example presented in this paper does not use the

environment concept at all. The interactions among actors simulate event-broadcasting (Harel & Politi, 1998) so as to reproduce cause-effect relationships. A different solution would have been introducing the *environment* component which is informed of significant changes in actors and propagates this information to interested actors. The environment can be realized according to different organizations.

Taking for example the viewpoint of HLA, a distributed system partitioned into N application theatres, each housing a given number of actors, could be really constructed along one of the following schemes:

- using N+1 theatres/federates, where the extra federate is dedicated to the centralized and shared environment component;
- partitioning the environment among the N federates so that each federate hosts the local portion of the environment accessed by local agents.

The first solution could be implemented into HLA by using the publish/subscribe architecture and by resorting to RTI ownership management for ensuring mutual exclusion on shared environment attributes. The solution, though, could suffer from computational degradation resulting both from centralization and ownership management.

The second solution (see also (Cicirelli *et al.*, 2009)) can be preferable but introduces problems at the boundary of adjacent theatres, also considering that the solution must face agent migrations.

Environment organization is an open and important issue in general multi-agent systems. It will be investigated also in the light of the interesting work of "spheres of influence" described in (Logan & Theodoropoulos, 2001).

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SINCITY: A PEDAGOGICAL TESTBED FOR CHECKING MULTI-AGENT LEARNING TECHNIQUES

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KEYWORDS

Multi-agent learning, urban traffic models, NetLogo.

ABSTRACT

In this paper we present SinCity, a pedagogical testbed to compare multi-agent learning strategies. SinCity has been developed in NetLogo and it can be considered as an extension of the simple predator-prey pursuit problem. In our case, we model a police/thief pursuit in an urban grid environment where several elements (cars, traffic lights, etc.) may interact with the agents in the simulation. SinCity allows to model, in a graphical friendly environment, different strategies for both, the Police and the thief, also implying coordination and communication among the agent set. SinCity is oriented mainly as a pedagogical testbed for learning techniques. The main contributions of the paper are a graphical simulating environment in NetLogo (distributed as open source), a pedagogical testbed for simulating multiagent learning strategies, and the results concerning the simulations performed.

INTRODUCTION

The predator-prey pursuit problem (Benda et al. 1985) is one of the first and well-known testbed for learning strategies in multi-agent systems. Basically it consists in a set of agents, named predators, that aim to surround another agent, named prey, that must escape from them. This problem has been addressed many times by the AI Community. Initially, (Korf 1992) proposed a solution without multi-agent communication. A great number of alternatives have emerged since Korf's one, involving genetic programming (Haynes and Sen, 1995), Petri nets (Chainbi et al. 1996), reinforcement learning (Tan 1997), blackboard architectures (Jim and Giles, 2000), profit sharing (Katayama et al. 2005), and many more.

Many other learning simulations have appeared in multiple domains (social sciences, economy, biology, ecommerce, etc.) and with much more complex scenarios. Presently one of the most popular ones are the Robocop Simulation Leagues for Soccer and Rescue (Robocop 2006). The simulators and techniques used for these two competitions are brand new approaches but usually very complex to be managed as a

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) pedagogical testbed for comparison of new learning techniques.

In this paper we propose a simulator named SinCity, modeling a city, and a new pursuit problem, which is a more complex version of the predator-prey. SinCity is developed in an open source, simple, popular and user friendly environment (Netlogo) that may be used as a testbed for checking multiple multi-agent learning techniques.

The rest of the paper is organized as follows. First we introduce multi-agent systems and the Netlogo environment for multi-agent simulation. Then we describe the simulation scenario developed. Next, we introduce our police-thief pursuit model. In next section we describe the learning techniques used in our simulations and the results we have obtained. Finally, we present the conclusions and future research work.

MAS AND NETLOGO

In this section we introduce Multi-agent Systems (MAS) and Netlogo, which are the basic elements used to build the SinCity simulator.

Multi-agent Systems

Before introducing Multi-agent Systems (MAS), we need to define what we understand by an agent. Unfortunately, there is no general agreement in the research community about what an agent is. Therefore we cite a general description (Wooldridge and Jennings, 1995), and according to it, the term agent refers to a hardware or (more usually) software-based computer system characterized by the well-known properties: autonomy, social ability, reactivity, and pro-activeness. There are some other attributes that can be present, but usually they are not considered as a requisite: *mobility*, veracity, benevolence, rationality and adaptability (or learning); see (Wooldridge 2002) for more details. A system consisting of an interacting group of agents is called a Multi-agent System (MAS), and the corresponding subfield of Artificial Intelligence (AI) that deals with principles and design of MAS is called Distributed AI.

Netlogo

We implemented our city model using NetLogo (Wilensky 2007), a multi-agent modeling environment for simulating natural and social phenomena. It is particularly well suited for modeling complex systems that evolve. Modelers can give instructions to hundreds of agents operating independently. This makes possible to explore the connection between the micro-level behavior of individuals and the macro-level patterns that emerge from the interaction of many individuals.

NetLogo is an easy-to-use development environment. It allows to launch simulations and play with them by exploring their behavior under various conditions. Custom models can be created easily for quick tests of hypotheses about self-organized systems.

NetLogo has extensive documentation and tutorials. It also comes with a Models Library, which is a large collection of pre-written simulations that can be used and modified. These simulations address many areas in natural and social sciences, including biology and medicine, physics and chemistry, mathematics and computer science, and economics and social psychology.

NetLogo is a 2D world made of agents that simultaneously carry out their own activity. There are three types of agents:

- Patches: stationary agents that make up the background or "world". They have integer coordinates.
- Turtles: mobile agents that move around on top of the patches, not necessarily in the center, so they have decimal coordinates and orientation.
- The observer: oversees everything going on in the world. It can create new turtles and has read/write access to all the agents and variables.

An agentset can be created using a subset of the agents. There is also the possibility to create breed, a "natural" agentset of turtles, which come with automatically derived primitives.

NetLogo uses a simple scripting language to define the systems, and it also has a user-friendly graphical interface to interact with the system. The graphical interface consists of three elements:

• Controls: they allow to run and control the flow of execution. There are two types: buttons and command center. The buttons are used to initialize, start, or stop the model, and step through it. They can be either "once", which execute one action (a piece of code) or "forever", which repeat the same action (the same piece of code) until pressed again. The command center allows to ask observer, patches or turtles to execute specific commands "on the fly", while the model is running, so it is

possible observe how these modifications alter the model.

- Settings: they allow to modify parameters. There are sliders (to set a quantity from a minimum to maximum by incremental steps), switches (to set a boolean variable true or false) and choosers (to select a value from a list).
- Views: they allow to display information. There are monitors (to display the current value of variables), plots (to display the history of a variable in a graphic), output text areas (text log information) and graphics window (main view of the 2D NetLogo world).

As common programming languages, NetLogo has variables, i.e., value containers. There are global variables (a single value for the variable that every agent can access it), turtle and patch variables (each turtle/patch has its own value for every turtle/patch variable), local variables (defined and accessible only inside a procedure) and built-in variables (already defined in NetLogo for turtles and patches).

To model the behavior of the agents, NetLogo has different procedures: commands (actions for the agents to carry out, i.e. "void" functions), reporters (to report a result value, i.e. functions with return type), primitives (built-in commands or reporters, i.e. language keywords), procedures (user-made custom commands or reporters) and "ask" (to specify commands to be run in parallel by a set of turtles or patches).

CITY MODEL

Previous models

The first approach to traffic models, which is included in the NetLogo distribution, is Traffic Basic (Wiering et al. 2004) (figure 1). It models the movement of cars on a highway. Each car follows a simple set of rules: it slows down (decelerates) if it sees a close car ahead, and it speeds up (accelerates) if it does not see a car ahead. It demonstrates how traffic jams can form even without any "centralized cause".



Figure 1: Traffic Basic Model

Using the movement of the cars in the previous model, a small city with traffic lights is modeled in Traffic Grid (Wilensky 2005) (figure 2, left), also included in the NetLogo distribution. It consists of an abstract traffic grid with intersections between cyclic single-lane arteries of two types: vertical or horizontal. It is possible to control traffic lights, speed limit and the number of cars, creating a real-time traffic simulation. This allows the user to explore traffic dynamics and develop strategies to improve traffic and to understand the different ways to measure the quality of the traffic.



Figure 2: Traffic Grid (left) and SOTL (right) Models

Using the Traffic Grid model as a starting point, a more complex model is presented in (Gershenson 2004), called Self-Organizing Traffic Lights. Cars flow in a straight line, eastbound or southbound by default. Each crossroad has traffic lights that only allow traffic flow in one of the arteries that intersect it with a green light. Yellow or red lights stop the traffic.

The light sequence for a given artery is green-yellowred-green. Cars simply try to drive at a maximum speed of a "patch" per time step, but they stop when a car or a red or yellow light is in front of them. Time is discrete, but space is continuous. A "patch" is a square of the environment with the size of a car. The environment is shown in figure 2 (right). The user can change different parameters, such as the number of arteries or cars.

Different statistics are shown: the number of stopped cars, their average speed, and their average waiting times. In this scenario, the author presents three selforganizing methods for traffic light control outperforming traditional ones, since the agents are "aware" of changes in their environment, and therefore they can adapt to new situations.

City Model Improvements

Our model is a more realistic city scenario, as we will explain in this section. To model the 2D scenario, different agentsets for the patches are used. The main ones are:

- intersections: agentset containing the patches that are intersections of two roads.
- controllers: agentset containing the intersections that control traffic lights. Only one patch per intersection.
- roads: agentset containing the patches that are roads. The rest of the patches are buildings. There will be four sub-agentsets, depending if the road is southbound, northbound, eastbound or westbound.

- exits: agentset containing the patches where cars will go when leaving the simulation.
- gates: agentset containing the patches where cars will sprout from.

Given the previous model of the traffic in a city, described in [10], we have made some improvements to represent a more realistic scenario. In the previous model, the roads have a single lane and direction, and there are only two directions by default, south and east, although they can be changed to four, by adding north and west. A car only changes road or direction depending on a probability prob-turn, which means that the cars move at random. Also, in the previous model a torus was used by default, which means that when a given car coming from the west to the east arrives to the end of the scenario at the east, the same car will appear at the beginning of the scenario at the west.

To increase realism, we remove the torus and impose four directions (north, east, south and west), and we are able to shape traffic thanks to sliders *vertical*, *southbound* and *eastbound*. Also, a by-pass road is created to improve traffic, which is the outermost in the scenario.

We have also changed the car creation and elimination scheme. Now, for every car, we define a source (a random road patch) and a destination (another random road patch), such that every car is created at a source, and it moves (following the shortest path) to its destination, where it is eliminated. The sources and destinations may be outside the world, depending on the value of the sliders *origin-out* and *destination-out*, leading to some cars appearing and disappearing at the borders of the world.

We have added the possibility of bidirectional roads, which are controlled with slider *bidirectional*, and roads with two lanes in the same direction, controlled with slider *2-lane*.

We have modified all the control methods so that, instead of just one yellow light cycle, now there are as many yellow light cycles as patches in the intersection, i.e. if the traffic light protects a bidirectional road, with two lanes in each direction, there will be four yellow lights cycles. In order to try to correct deadlocks at the intersections, a deadlock algorithm has been implemented. If a given car at an intersection after a given time has not moved, it tries to change direction in order to keep moving and to try to exit the deadlock. This movement could affect other cars and help finishing the current deadlock.



Figure 3: The SinCity Model

Due to all these improvements, specially the possibility of an origin and a destination and bidirectional roads, a complex algorithm to guide the cars is needed. Whenever a car is in a patch that is an intersection (it belongs simultaneously to a horizontal and a vertical road), it runs the guiding algorithm in order to know if a change of direction is necessary, before moving on. If not, the car will keep the same direction, at least until the next intersection.

As seen in figure 3, with these changes we obtain a more realistic scenario where we can notice the different widths of the streets, depending if they are bidirectional and single or dual lane streets. We can also see the distribution of the traffic lights, and the by-pass road surrounding the city.

THE SINCITY PURSUIT MODEL

Our SinCity simulation is an extension of the predatorprey pursuit problem, where the prey is substituted by a thief car and the predators by a set of police cars.

On every challenge, the thief car starts driving at normal speed to a city bank. It stops in front of the bank, does the theft and getaway to its hideout at double speed. On the other hand, police cars patrol the city before the theft is done. When the thief car robs the bank an alarm is triggered, and police cars double their speed and patrol along the city trying to identify the thief's car. The chase begins when any police sees the thief, before it arrives to its hideout, in the same road and at a distance of two blocks or less. On the one hand, if the thief's car is seen, then all police cars know its position. On the other hand, if it is lost, we keep the point where the thief was last seen. If any police car arrives to that point but the thief car is not in sight, then the chase stops, prevent the others to go to that place and the patrol continues.

We consider that the thief is captured if it is surrounded by police in a road (two police cars) or in an intersection (4 police cars). We consider that the thief escapes when it reaches its hideout and enters into it without to be seen by any police car. Besides, there are more cars in the city that cause thief or police cars to reduce their speed in the prosecution, from double to a normal one, if they are in front of the car.

Figure 3 shows a snapshot of the SinCity map and data with the thief car is highlighted. The bank is marked in red at the upper right and the hideout is marked in green at the center. At every challenge the position of the bank and hideout changes but they must have a distance greater than the 25% of the map size. At the bottom and the right of the map we can see a graphic display, some outputs related with the simulation, and also configure several parameters; related with the algorithms explained in next sections.

ALGORITHMS AND LEARNING TECHNIQUES

In this section we describe the learning techniques implemented in the SinCity simulator to compare their results. We have implemented the non-learning Korf's Algorithm, a self-organizing neural network (SOM) and two reinforcement learning algorithms: Learning Automata and Q-Learning. All these techniques are described next.

Korf's Algorithm

(Korf 1992) approach was to use a fitness function that combined two forces: each predator was "attracted" by the prey and "repelled" from the closest other predator. This solution kept predators away from other predators while they got closer to the prey; the idea was to chase the prey arranging predators in an stretching circle. Korf concluded that the pursuit domain was easily solved with local greedy heuristics.

Self-Organizing Maps Algorithm

A Self-Organizing Map (SOM) (Kohonen 2001) is a type of artificial neural network that is trained using unsupervised learning to produce a low-dimensional (typically two dimensional), discretized representation of the input space of the training samples, called a map. We use the formula:

$$Wn(t+1) = Wn(t) + \Theta(t) \cdot \alpha(t) \cdot (I(t) - Wn(t))$$

where $\alpha(t)$ is a monotonically decreasing learning coefficient and I(t) is the input vector. The neighborhood function $\Theta(t)$ depends on the lattice distance between the winner neuron and neuron v.

Learning Automata Algorithm

The Learning Automata (Narendra and Thathachar, 1989) is a type of reinforcement learning algorithm that uses two very simple rules:

$$P(s,a) = P(s,a) + \alpha . (1 - P(s,a))$$
(1)

$$P(s,b) = (1 - \alpha) . P(s,b)$$
(2)

In these equations (α) is a small learning factor. If case of success, rule (1) is used to increase the probability of action (a) in state (s), while rule (2) is used to decrease the probability of the rest of actions.

Q-Learning Algorithm

The Q-Learning algorithm is another type of reinforcement learning algorithm (Kaelbling et al. 1996), which works with the well-known formula:

$$Q(s,a) = Q(s,a) + \alpha \left(R(s) + \gamma \max_{b} Q(s',b) - Q(s,a) \right)$$

Where (s) is the previous state, (s') the next state, (a) the action previous chosen, (α) the learning factor, (R(s)) the reinforcement, (γ) the discount factor, Q(s,a) is the value of Q for the present state and action chosen, and Q(s',b) for the next state (s') and action b.

SIMULATION RESULTS

In this section we present our simulation conditions and results. The simulations have been performed on a superserver with 8 processors Intel(R) Xeon(R) CPU X5460 at 3.16GHz and with 6 MB of cache memory per processor taking less than an hour for the whole set. We use a 65% of bidireccional roads and we generate a new city for every challenge.

For implementing the learning techniques described in the previous section we took several decisions. First, police cars and the thief car take decisions about what road to take only at every intersection. This reduces the number of states and speed up the simulations.

The thief has two different learning systems. The first is used to go from its particular location to the hideout when there is no police car at sight. The other learning system is used in the chase to escape from the police. The police car only have one learning system which is used to go from its present location to a destination, for instance, to pursue the thief during the chase.

For the LA and QL techniques, when going to a destination, the input for every learning system considers the possible configurations of the road intersection (16 - 1 = 15 possibilities, as one has all roads blocked) depending if a certain road is blocked or not. We also consider the 8 possible locations of the destination point around the car. Therefore we have 8 x 15 = 120 input states for LA and QL.

In the thief case, using LA and during the chase, we consider only what is the closest police car. Therefore we have 4 inputs x 15 possible road intersections = 60input states. For the QL case, we consider the discrete distance in blocks (0, 1 or 2) of every police car when they are closer than two blocks. Then we have 81 inputs x 15 road intersections = 1215 states. Finally, the SOM neural network is only used by the thief during the chase. First we identify the type of intersection we have (15 possibilities) and for each one we set a SOM with 4 real valued inputs (the 4 directions) with a number describing the exact distance to a police car (if anyone if less than 2 blocks, or zero if there is no one). We used a lattice of 16 x 16 = 256 neurons. Therefore, we have $256 \times 15 = 3840$ neurons with 4 inputs each one. The output of every neuron is one of the four possible roads to take and it is based in a probability distribution of those possible exits, and trained as the LA case.

The learning parameters we used in the simulations are: α =0.1 for the LA, QL and the probability distribution of every neuron in the SOM. Besides, in QL we set R(s)=±0.25 and γ =0.2. Finally, for the SOM case we have (t) = 1 / (1 + 0.01*t) and $\Theta(t) = (t) = 1 / (1 + 0.01*t)$, where t is the learning iteration. Of course, as there are several SOMs, each one has its own (t) and (t) parameters.



Figure 4: % of thief victories using LA (2 police cars)

Figure 4 shows the evolution of the absolute percentage of thief victories along 1800 challenges in a city of 5x5 blocks; with the thief using the LA technique. We see how it starts low and it grows as soon as the automata learns the best options in every situation. After 1000 challenges, this percentage remains stable around 28%.

Now we compare the results using the learning techniques in a run. A run (set of challenges) stops when the average standard deviation of the thief wins in last 500 challenges is lower than a 3%, provided than at least 1000 challenges have taken place.



Figure 5: 10x10 map results with Police using Korf

Figure 5 shows the results obtained with a city of 10x10 blocks. We set the Korf's algorithm for the police cars and then we change the algorithms for the thief car. Korf's algorithm does not learn and may be used to compare thief success when using the learning techniques. As we may see in figure 5, the best results are obtained in average by the LA algorithm, followed by the Korf, SOM and the QL algorithms. This is even more interesting considering that the LA algorithm only uses less states and considers if there are police cars in a direction, but without determining their precise distance. We are still considering this curious result as

we see how sometimes an excess of information can be a disadvange, and simple solutions are good enough for complex problems; (Korf, 1992; Gershenson, 2004) exemplify it. As it was expected (figure 5) the percentage of thief victories decreases when the number of police cars increases.

We present in table 1 a comparison among the 3 learning strategies. LA is clearly the winner in all cases, and on the other side, QL obtains the worst results. We point out that SOM is only used by the thief.

Table 1:	% of thief victories amo	ng the learning
strategies: 1	LA, QL and SOM (used	only by the thief)

Thief Algorithm	Police Algorithm	Police Cars	% Thief Wins
LA	QL	2	81,4
SOM	QL	2	76,6
SOM	LA	2	59,4
QL	LA	2	48,2
LA	QL	4	77,2
SOM	QL	4	46,8
SOM	LA	4	34,2
QL	LA	4	20,4
LA	QL	6	60,2
SOM	QL	6	29
SOM	LA	6	18,2
QL	LA	6	10,4

CONCLUSIONS AND FUTURE WORK

In this paper we have presented SinCity, a simulating testbed that has been created to obtain a highly flexible and efficient testbed for MAS. SimCity has been developed in NetLogo and it can be considered as a more complex version of the predator-prey pursuit problem. In our case, we model a police/thief pursuit in an urban grid environment where other elements (cars, traffic lights, etc.) may interact with the agents in the simulation. SinCity allows to model, in a graphical friendly environment, different learning strategies for both, the police or the thief.

The main contributions of the paper are a graphic city simulator in NetLogo (distributed as open source), which serves as a testbed for simulating multi-agent learning strategies. We also present the results of the simulations performed.

As future work we plan to extend the model of the traffic in the city and to allow more complex interactions among the normal traffic and the police-thief cars. We also plan to implement more complex learning techniques and consider evolutionary programming techniques for generating the agents decision rules.

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Discrete Event Modelling and Simulation in Logistics, Transport and Supply Chains

SIMULATION OF MEDICAL LABORATORY OPERATIONS TO ACHIEVE OPTIMAL RESOURCE ALLOCATION

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Health care, discrete-event process simulation, resource allocation, route optimization.

ABSTRACT

As competitive pressures increase within the health care sectors of economies worldwide, and especially within the United States, the importance of achieving operational efficiencies to reduce costs and thence to increase profits while keeping and attracting customers steadily increases. Simulation, optimization, time value stream mapping. studies. and process improvement methodologies have long been key allies of the industrial engineer assigned to find and progress along the often difficult and challenging road leading to such efficiencies; experienced industrial engineers know these methodologies work better synergistically than individually. The presentation here, and undertaken collaboratively between the medical laboratory (client) and the industrial engineering service company (consultant), concentrates primarily on the use and achievements of discrete-event process simulation and its allied industrial-engineering techniques in improving the operations of a medical testing laboratory, and hence its services to its clients, both hospitals and clinics.

INTRODUCTION

Historically, the first major application area of discrete-event process simulation was the manufacturing sector of the economy (Miller and Pegden 2000). With the passage of time, simulation has become more closely allied with other industrial engineering techniques such as time and motion studies, value stream mapping, ergonomics studies, and "5S" examinations used concurrently to improve generic operations (Groover 2007), and has also expanded rapidly into the service and health care industries (Lowery 1998). Illustrative examples of simulation applications to the health care sector appearing in the literature are: improvement of appointment scheduling in a dental clinic (Czech, Witkowski, and Williams 2007), the analysis of incentives and scheduling within the operating room of a major metropolitan hospital (Ferrin et al. 2004), the coordinated provision of emergency medical services immediately subsequent to a serious traffic accident (Guimarans et al. 2006), and aggressive efforts to improve health care delivery in hospitals in the United Kingdom (Pidd and Günal 2008). The survey article (McGuire 1998) provides an excellent overview of simulation use in health care.

Improvement of the delivery of health care services is especially pressing in the United States. As Margaret Brandeau bluntly stated in her keynote address to the 2008 Winter Simulation Conference (Miami, Florida, United States, 8 December 2008) "The United States spends more per capita on health than any other nation, vet has worse health outcomes than many other countries. Moreover, expenditures on health in the U.S. are growing rapidly, and are taking up an increasingly larger share of per capita gross domestic product." (Brandeau 2008). These urgently needed improvements involve the metrics of timeliness, quality, and cost - and these metrics are strongly affected by services the typical patient does not "see" (Galloro, 2008) – such as those provided by medical laboratories. The recent work of (Chinea, Rodríguez, and González 2009) provides an excellent synopsis of simulation used in hospital resource management.

In the case study discussed here, a medical laboratory in the eastern part of the United States, sought to improve its financial efficiency, operational efficiency, and service to its clients. Accordingly, this laboratory undertook to use, with the collaboration and guidance of an industrial engineering consulting company, the techniques of industrial engineering, including discrete-event process simulation. This certified and accredited laboratory provides, over a multi-county area, pick-up and delivery courier services for supply requests, medical specimens, test result reports, and medical supplies. In this context, the project goals of the client laboratory were to:

1. Optimize the numerous courier routes to improve transport efficiency, particularly to deliver work (i.e., medical specimens to be analyzed) to the laboratory earlier in the work day. In the specific context of this simulation project, an ongoing, formally stated objective was (and is) "test impact of route optimization initiative on load leveling of resources and provide necessary feedback for

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further fine tuning of optimization model." Hence very early in the life of this project, the client recognized the first phase of the simulation study as a "bootstrap" toward continuous improvement (usually this recognition dawns later, after a client – especially one new to simulation – comes to appreciate the analytical power of simulation).

- 2. Gain analytical insights into the interrelationships between courier route improvements and operational performance metrics of the laboratory itself.
- 3. Achieve leveling of workload, in conjunction with leveling of resource usage, within various departments (e.g., serology, microbiology, and hematology) departments in the laboratory via smoother delivery of work.
- 4. Achieve cost-savings via appropriate redeployment of personnel with no degradation of service metrics to hospitals and clinics (the clients of the laboratory).

OVERVIEW OF PROCEDURES AT THE MEDICAL LABORATORY

The operations studied intensively and comprehensively at this laboratory comprised the delivery of medical specimens to the laboratory, their processing within the laboratory, pick-up and delivery of items entrusted to its courier service, and delivery of test result reports and medical supplies to its client hospitals and health care clinics. At the initiation of the project, the laboratory used a fleet of fifteen courier employed vehicles, fifteen full-time-equivalent headcount, and ran eleven total courier routes daily (only one of these a local run). Originally, courier routing instructions were handwritten on route sheets. Also, the laboratory was acutely aware of chronically high specimen processing costs, due primarily to overtime attributed to unbalanced rates of specimen arrival. The arrival rates predictably spiked about 11:30 each morning, between 14:00 and 17:00 each afternoon, and again at 22:00 each evening. The number of requisitions processed was typically between 1,000 and 1,100 per day. Unbalanced rates of specimen arrival resulted in suboptimal utilization of medical technologists. Overtimes were frequently enforced, in addition to the implementation of a midnight shift, to achieve required turn-around-time of 24 hours. Early observations and discussions with the client attributed this undesirable situation to suboptimal workload leveling. Additionally, unobtrusive workload observation techniques confirmed a long-standing client suspicion that between $\frac{1}{2}$ and $\frac{3}{4}$ hour of courier time was typically squandered between specimen drop-off and route continuation. As so often happens (Kroemer and Grandjean 1999), stressful working conditions, including compulsory overtime, often resulted in erroneous specimen results. Accordingly, the client and the consultant decided to concentrate early efforts on improvement of the courier routings and assignment of personnel thereto, not operations within the testing laboratory itself.

DATA COLLECTION AND INPUT ANALYSIS

A major portion of the data collection involved the courier routes; actual trip times (which had high variability) were collected and analyzed for each route. This need for extensive, accurate data collection is frequent in simulation studies, especially those pertaining to the health care industry. As (Carter and Blake 2004) remark, "In our experience in health care, no one ever had the right data in the form that we needed it." In this study, data collection included not only the routing details mentioned above, but the resource availabilities of couriers by shift, the proportions of specimens requiring attention in the chemistry, hematology, microbiology, and serology subdivisions of the laboratory, and staffing levels in each of these divisions. Additionally, all incoming specimens required generic preprocessing before being routed to one or more of the laboratory subdivisions; input data were also collected to assess the workload imposed by this preprocessing.

CONSTRUCTION, VERIFICATION, AND VALIDATION OF THE SIMULATION MODEL

Construction of the simulation model began concurrently with the collection and statistical analysis of its input data. The simulation software tool chosen in consensus by the client and the industrial engineering company was Enterprise Dynamics® (Hullinger 1999). This software tool, a worthy competitor among many, provides comprehensive analysis techniques, a convenient user interface, excellent three-dimensional animation, and provision for modelers to construct customized reusable "atoms" (Swain 2007). For the convenience of both the modelers and the client's management, the simulation model was constructed to read its input data from Excel® workbooks and to export its numerical results to Excel® workbooks.

The scope of the simulation model included the courier team's acquisition of specimens, their preprocessing on delivery to the laboratory, their subsequent routing to specialized analytical operations (chemistry, hematology, microbiology, and serology), and the delivery of results and any requisitioned medical supplies to the client hospital or clinic. In the model, all courier routes were "black-boxed," i.e., treated as an advance of time sampled from the distribution of actual trip times collected for each pertinent route. Additionally, and with client concurrence, weekends were not modeled, and operator walk times and lunch breaks were ignored.

Verification and validation of the simulation model used many techniques well recognized in the literature (Sargent 2004), such as:

- 1. Running the model with only one entity.
- 2. Running the model with only one courier route.
- 3. Eliminating all randomness and then crosschecking results against "desk arithmetic."
- 4. Using structured walkthroughs of model logic and code.
- 5. Undertaking "directional testing" (e.g., if a cycle time increases, throughput should decrease or remain the same).
- 6. Cross-checking extensively with the client, including step-by-step tracking of model execution and its animation.

Availability of three-dimensional animation proved of ongoing value when the results were presented to client engineers and those engineers in turn presented them to their upper management (Kelton, Sadowski, and Sturrock 2007). An example of a three-dimensional animation appears as Figure 3 in the Appendix. Likewise, the availability of interactive route maps interfaced with the simulation analysis, one of which appears in Figure 4, were a valuable visual aid to understanding the implications of various suggestions for routing improvement.

RESULTS AND OPERATIONAL CONCLUSIONS

The results of this simulation study included several pertinent and valuable recommendations, among them:

- 1. Optimizing routes initially in use allowed the reallocation of two couriers.
- 2. One re-allocated courier, redeployed as a runner, retrieved specimens from other couriers returning to the site.
- 3. Workload leveling achieved as a result of optimizing the routes helped the client eliminate the night shift and improve utilizations of medical technologists during the morning shift. One example of workload leveling achieved is illustrated in Figures 1 and 2, which show the percent utilizations of the medical technologists in the chemistry department. Resource leveling improved from "considerably worse than two-toone" to "uniformity of usage within 10%." Similar quantitative improvements were achieved in the serology, microbiology, and hematology departments.



Leveling, Chemistry Department



Figure 2. Resource Utilization <u>after</u> Load Leveling, Chemistry Department

A lesser ratio improvement, but one involving a more heavily utilized group of technologists overall (and hence of high importance to the client) was achieved in the preprocessing department, as shown in Figures 5 and 6 in the Appendix. In this department, maximum utilization fell from 100% (and that among half of the technicians) to 97%, and minimum utilization rose from 60.2% to 81.7%.

4. Route optimization and subsequent workload leveling saved approximately \$110,000 annually in payroll costs.

It is important to understand that the progress from optimization of courier routes to achievement of workload leveling was not a quick "step one, step two" process. The actual work involved improving the courier routes, testing the impact of these improved routes on workload leveling, using insights from the newly improved leveling to further improve the routes, etc. – an iterative process. Relative to the simulation experimentation itself, the scenario runs were terminating (due to the daily "restart" nature of the courier runs and laboratory operations), each replication lasted six weeks of simulated time, and sufficiently narrow confidence intervals required four replications of each scenario examined.

Attractively, no personnel represented by the payroll cost savings were laid off; rather, the client company deployed them in expansions of this service and in newly offered services, thereby increasing its profitability. As one example of this reallocation, one courier was newly deployed as a runner assigned to retrieve laboratory specimens, together with handheld computers already in routine use to upload preliminary computations to desktop computers, from other couriers returning to the central laboratory from their runs.

INDICATED FURTHER WORK

As a matter of standard policy, the model was built and documented with the intention that it be available for and adaptable to continued use. Such continued use is indeed already impending: almost inevitably, changes in the number and location of customer pickup/drop-off points are appearing, as are changes in the "specimen traffic" (number of specimens arriving or departing at each of these points). Therefore, courier routing optimization will be an ongoing process. Via the Excel® input interface, client analysts and managers can and do run the model to incorporate these changes, the routing optimization is successfully keeping apace of the market demand changes experienced by the laboratory.

Additionally, as a result of a first successful foray into simulation by the client company, its management is now considering the use of simulation for an incremental study focusing attention more specifically on the "in-house" laboratory operations.

OVERALL CONCLUSIONS AND IMPLICATIONS

This case study illustrates the value of simulation in a setting fundamentally logistical, in the context of providing health care. Use of simulation in conjunction with allied analytical techniques such as route optimization, value stream mapping, work sampling, and resource leveling provides synergistic value to all these industrial engineering techniques. Whereas many studies documented in the literature are directed to the "front of the house" delivery of care directly visible to patients, this analysis devoted attention to a "back of the house" function, much less conspicuous from a patient's viewpoint, but nonetheless vital to the delivery of timely and high-quality health care at manageable cost.

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APPENDIX



Figure 3. Three-dimensional Animation of Laboratory Processing



Figure 4. Route Map Interfaced with the Simulation Analyses



Figure 5. Pre-Processing resource utilizations before load leveling



Figure 6. Pre-Processing resource utilizations after load leveling

A DYNAMICAL MODEL FOR THE AIR TRANSPORTATION NETWORK

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KEYWORDS

LT: Discrete Event Modelling and Simulation in Logistics, Transport and Supply Chains

ABSTRACT

Although in the literature several Air Transportation Networks have been modeled through the mathematical framework of Complex Networks, less attention has been devoted to their evolution: specifically, topology is studied as static, excluding any schedule information. Simulating the growth of an air network is not an easy task, due to the great amount and heterogeneity of agents interacting (aircrafts, controllers and more). In this work we use a recently developed tool, called Scheduled Network, to define an algorithm to simulate such a growth; the basic assumption is that the cost for passengers should be minimized, which is approximated with the time needed to go from one airport to another one. Some results are presented, and the role and importance of hubs (that is, central airports where great part of the flights are concentrated) is discussed.

INTRODUCTION

The Air Transportation Network has been rapidly evolving in the last decades, mainly due to the many technological changes introduced: more efficient aircraft have modified any previous business perspective, giving birth for instance to low-cost airlines. The increment in the number of operations, and the consequent need for optimal investment strategy, is a significant challenge for regulation and control authorities: for example, Eurocontrol is forecasting a growth of up to 220% in the number of flights inside Europe in the time window 2005 - 2030(STATFOR, 2008).

Intuitively, the study of the structure of this network and the forecast of its evolution are extremely valuable tools for policy makers: but indeed are not easy tasks, due to the great number of agents interacting and to the complex interactions between them. Inside the Complex Science paradigm, we have chosen an instrument which simplifies that task, and we have adapted it to this context: that is, Complex Network theory.

Complex Networks are mathematical objects with a simple definition (Boccaletti et al., 2006; Newman, 2003): nodes (which represent any kind of physical or virtual entities) connected through links (once again, any kind of relations) following a given topology. Exploiting this generality, many studies of the structure of real and virtual systems (Costa et al., 2008), and properties of such topologies (Costa et al., 2007) have been proposed.

Although powerful, this network framework has an important drawback: the structure is considered as static, and does not include any time evolution. Let us show an example of how this can lead to some problematic consequences. In a previous work, Guimerà (Guimerà et al., 2005) constructed the network of worldwide flights by connecting two cities if there were a direct flight connecting them; no information regarding flights duration or allowed concatenations is therefore taken into account. For instance suppose that a customer has a flight at 12:00 from Stockholm to Paris, and another flight the same day from Paris to Toulouse at 13:00; clearly we cannot claim that Stockholm and Toulouse are connected in that time window by a path of length 2, as the passenger would be flying at 13:00 and would miss the second plane: he/she will have to wait until the next flight, maybe the following day.

To overcome this class of problems, an extension of Complex Network which includes the time scheduling has been developed by the authors (Zanin et al., 2009). This Scheduled Networks approach allows dynamically activating links according to an external source of information: as a consequence, it is possible to directly study its topology and extract useful information, as mean rotation times and system efficiency.

In this work, we have applied Scheduled Networks to several virtual air networks with the aim of forecasting their evolution. Initial conditions are defined as airport positions and flux of passengers between them: after that, links (that is, flights) are sequentially added to minimize an objective function which represents the cost for customers to travel across the network. The remainder of the work is organized as follows: first, an introduction to the mathematics of Scheduled Networks is presented; after that, several virtual networks are constructed, and some conclusions about the behavior of such systems is discussed.

SCHEDULED NETWORKS

The first step to construct an algorithm for simulating the growth of air traffic networks is to define an extension of Complex Networks which includes a time schedule. So, we start with the definition of a static directed network,

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Figure 1: (Left) Representation of a simple directed network, which has been expanded (Center) to include a representation of time (i.e. the time needed to travel along a link). At the Right, both connections of the network are deactivated, by deleting the first link of each path.

where *n* nodes are connected through links; those connections are represented in an *adjacency matrix* $A_{n \times n}$, where the element a_{ij} has a value of 1 if there exists a link between nodes *i* and *j*, and zero otherwise (Bollobas, 2002).

This structure is now transformed to include the time needed to travel a connection, as shown in Fig. 1. To the primary nodes, which correspond to the original nodes of the graph, some secondary nodes are added, that are used to delay movements according to the scheduling information. Those secondary nodes are virtual, as they do not exist in the real system under study, and represent the time length of each link. The new adjacency matrix is now the combination of a differential adjacency matrix dA, which is constant and represents one time step, and an Activation Matrix, which holds the scheduling information. The global adjacency matrix, and therefore dA, is a square matrix of $n \times n$ elements, where n is the sum of primary and secondary nodes $(n = n_p + n_s)$. To simplify the notation, S is constructed so that the primary nodes are represented first, followed by secondary ones. This new adjacency matrix is divided into four parts, as in Eq. 1.

$$A = \begin{bmatrix} P & R \\ Act & T \end{bmatrix}$$
(1)

Within Graph theory, the adjacency matrix fully characterizes the set of allowed movements that a given agent can perform inside a network. In a similar way, each one of the four sub-networks has a specific function:

- Persistence matrix (P): is a $n_p \times n_p$ identity matrix, which allows agents in a primary node to stay there indefinitely.
- Activation Matrix (Act): this matrix represents the schedule of the network, and is dynamically updated at each time step. When a link is activated, agents are allowed to move from a primary node to the first secondary node of that link.
- Reception Matrix (R): it moves an agent from the last secondary node of a link to the primary node which is the end of the link.

• Transfer Matrix (T): this matrix moves agents in a secondary node to the next node of the same link, so that they can travel until the destination airport; in other words, it simulates the passage of time.

A deeper explanation of how to construct the new Adjacency Matrix can be found in (Zanin et al., 2009), while an example of the resulting structure of the network of Fig. 1 can be found in the following matrix - note that the link from B to C is activated:

It is easy to chain together several adjacency matrices, to represent a whole time window. The static adjacency matrix is the same in each time step, and just the Activation Matrix is updated following the given schedule. Mathematically, it can be expressed as:

$$A = A(t) \cdots A(t+\delta-1)A(t+\delta) =$$
(3)
=
$$\prod_{p=t}^{t+1} [dA + Act(p)]$$

In the original work (Zanin et al., 2009) this framework has been used to calculate several important metrics of the European Air Transportation Network, like efficiency and rotation time. Mathematics apart, now we want to simulate the growth of a virtual air network: and this tool helps us in creating a more realistic simulation by including the time dimension inside the system.

MODEL DEFINITION

Our model includes 9 virtual airports, placed in a regular lattice. Each airport is defined by two parameters: (i) the number of passengers that want to travel from that given airport, and (ii) a fitness, i.e. a value representing the relative attractiveness of that node for travelers. When both values are included in two vectors \overline{P}_i and \overline{F}_i , with $1 \leq i \leq 9$, the effective number of passengers going from node j to k is:

$$p_{j,k} = P_j \frac{F_k}{\sum\limits_{1 \le i \le 9, i \ne j} F_i}$$
(4)

In other words, the passengers that are ready to depart from one airport are distributed to the other 8 according to their attractiveness. As time is included in the system, it is necessary to define at which time of the day



Figure 2: Proportion of passengers traveling through the European Air Network as a function of the time of the day.

those customers want to travel; with that aim, we have extracted from real European traffic data an estimation of the mean number of passengers as a function of the hour of the day. Results are shown in Fig. 2, and have been included in all simulations.

At this point, it is necessary to define a target function for the system, which should be minimized (or maximized) when creating the network of connections. In real life, airlines have a clear mission: maximize the company value. Benefits are a complex combinations of incomes (flight tickets, airplanes renting, ...) and costs (airplanes depreciation, fuel, and so on); moreover, some companies (specifically, freighter airlines) have to dynamically rearrange connections to respond to customers' needs. With the aim of simplifying this complex space of variables, we have defined our function to be minimized as the cost for passengers to travel from a node to another, that is, the time required:

$$z = \sum_{i \in \mathcal{P}} T(i) \tag{5}$$

with P the group of all passengers, and T(i) the time needed by passenger *i* expressed in hours. This is a realistic approach, as airlines can charge passengers according to the usefulness of the flight (or of the group of connected flights), which is in inverse proportion to the duration. We also further simplify the system by only considering passenger transportation (that is, no freighter airlines), which networks are more static.

With all the above definitions, it is clear that the best solution would be a fully-connected graph; to impose some economical restriction to this problem, we limit the number of allowed flights for each graph (or the number of available airplanes), and we check the evolution of the system when this quantity is gradually increased.

The growing algorithm is therefore defined as follows. At the beginning airports are not connected; after that, at each time step, a new single flight is added to the system. To determine which connection has to be chosen,



Figure 3: Growth of the aeronautical network without any hub, and linear costs. In this case, the resulting topology depends only on the statistical fluctuations of the number of passengers in each airport.

all possible flights (that is, each possible pair of airports, and each possible hour of departure) are checked, and the one which minimizes the global cost is added - what is mathematically called a *greedy algorithm*. Of course, this algorithm wants to emulate a real situation where an airline has enough business volume and decides to add a new flight.

We have simulated two main situations:

- A regular lattice, where airports have similar number of passengers and fitness: only the geographical position is therefore defining the final network topology.
- 2. To the previous situation, a hub is added. In the aeronautical context, a hub is a central airport where most of the flights converge, and where maintenance is carried out. In our system, we have introduced such hub incrementing by 100% the number of passengers and the fitness of the central airport (Node 5 in all Figures).

SIMULATIONS' RESULTS

The result of growing the virtual aeronautical network described in the previous Section is shown in Fig. 3 and Fig. 4. To check the differences introduced by a hub, in Fig. 3 is shown the result for the first configuration (that is, all nodes have similar numbers of passenger and fitness); similarly, in Fig. 4 are shown four steps in the evolution of the second configuration, with a central hub: the evolution of the mean cost for this case is represented in Fig. 5.

Some considerations should be emphasized. First, in the case of Fig. 4 the emerging structure, at least for low number of connections, is an hub-and-spoke. This topology is usually defined as the best way to construct an aeronautical network, because with a limited number of flights all airports can be connected: of course, passengers have to take two different flights, one from the node of origin to the hub, and the second from the hub to the destination. Indeed this is the solution found by the growing algorithm; nevertheless when we further add connections, such star structure is lost, and many flights appear to link peripheral airports. In other words, what we have created in this simulation is a complex network



Figure 4: Growth of the aeronautical network with a central hub, and linear costs. Results are shown for 18, 30, 40 and 60 links.



Figure 5: Evolution of the mean travel time of passengers in a given node as a function of the number of links; the configuration considered is with a central hub and linear costs.

of connections, where peripheral flights are usually oper-



Figure 6: Growth of the aeronautical network with a hub in node 5 and quadratic costs.

ated by regional or low-cost airlines.

The question which may arise is what is the main reason to create a hub-and-spoke structure when few flights are allowed: the presence of a *natural* hub (i.e. a node with a higher volume of passengers), or its central position? The answer can be deduced from Fig. 3: when no node is artificially promoted to hub by increasing its traffic, the central position is not enough for node 5 to become a central airport.

In Figs. 3 and 4 we have supposed that the cost for users is a linear function of the time required for the trip (as in Eq. 5); to ensure that results do not depend on the form of the target function, we have also calculated the network evolution for a quadratic cost, in the form:

$$z = \sum_{i \in \mathcal{P}} T(i)^2 \tag{6}$$

With this new cost, results does not differ substantially and fewer links are needed to break the star topology (see Fig. 6). Of course, to create a more realistic simulation for real world air networks, it would be necessary to define a better economical approximation to the function which define the cost for users - or a better approximation of airlines benefits.

In order to check the robustness of obtained results, we have executed different simulations with noise in the flux of passengers. Obtained networks have similar characteristics; as may be expected, the regular structure is broken if the noise level is increased: see Fig. 7. Also, we have calculated the sensitivity of the solution of Fig. 4 with 30 links to noise applied to customers' fluxes; values of matrix P are now random variables with a normal distribution, centered in $p_{i,j}$, and whose standard deviation is the noise intensity. Results are shown in Fig. 8. It is worth noting the importance of such calculation when made in a real air transport network, as it would allow a quantification of the uncertainty embedded in the system.

CONCLUSIONS

From the above, some important informations can be inferred, which are of utmost importance for policy making and for the strategic planning of an airline.

First, the hub-and-spoke structure of connections, which is considered the standard configuration for an aeronautical network, is useful only as long as the number of flights is lower than a certain threshold: and this



Figure 7: Growth of the aeronautical network with a hub in node 5, linear costs and 18 links, when a strong noise is added to the matrix *P*.



Figure 8: Distribution of the obtained total cost when different noise levels are added to the matrix P, with the network configuration of Fig. 4. This represents the sensitivity of the system to random events.

situation can be found only in new markets. The reality is much more complex: regional airlines cover connections between non-hub airports, and low-cost companies try to dodge big airports to avoid high costs. The only way to take into account all those aspects is to construct a complex framework which allows a simulated growth of the network: this tool can indeed help in understanding the future evolution of the real air transportation system.

Second consideration: hubs appear as a consequence of the higher volume of passengers of some airports, and are not necessarily related with their physical position. This explains some interesting examples, like the hub of Munich, which is in the southern border of Germany. At the same time, it is not feasible to design a hub for political interests: if the selection is not supported by economical considerations in term of efficiency for passengers, it would be difficult for that hub to develop.

In further studies based on this model, we want to better understand the economical and geographical factors that can affect the choice of the location of a hub, and its role in the diffusion process. Moreover, the next step will be to apply this framework to real air networks, with the aim to forecast their evolution, as well as other factors: sensitivity to noise or random events, or uncertainty of the whole system. In turn this would allow a better planning of infrastructure investments and air structure modifications.

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STRUCTURAL COMPONENTS IN MULTIADJUSTABLE ROAD TRAFFIC MODELS: THEIR ROLE AND THE MEANS OF GENERATING THEIR TOPOLOGY

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KEYWORDS

Road traffic modeling and simulation, multiadjustable model, structural component.

ABSTRACT

This article presents advanced features of structural components in multiadjustable road traffic models. It shows that by making the structural components the active elements of the model, it is not only possible to enable multiple-level-of-detail modeling of traffic, but it also makes solving some corner-case situations much easier. Further, it deals with the problem of describing the topology of the traffic network that could be used for both macroscopic and microscopic structural components. It identifies a minimum set of information for such description and provides methods for deriving the remaining information from this minimum set.

INTRODUCTION

Modeling and simulation of road traffic has gained in popularity in recent years. This is not surprising, because it constitutes the only tool available so far for predicting behavior of a traffic system. Using traffic models, it is possible, for example, to evaluate the impact of the traffic restrictions related to a road work (whether construction or maintenance) and to determine which combinations of road works can be performed simultaneously without causing unnecessary congestion, or to compare the performance of several different road design alternatives. In connection with the recent onset of intelligent traffic management and information systems, traffic models can also be used to test these systems during their development in a real-like environment.

In our previous research (Zelenka, 2009), we proposed a general framework and a methodology for refactoring the structure of road traffic models to agility. We found that by introducing structural and behavioral components (see also the next section), it is possible to make use of component substitutability for easy changes in both structure and behavior of the models. Further, by making the structural components the active elements of the model and introducing component adapters, it is possible to simulate the traffic at different level of details in different parts of the model. Together, these two concepts lead to what we started to call multiadjustable models, because the features of such a model can be changed almost arbitrarily.

THE ROLE OF STRUCTURAL COMPONENTS

Today, there are basically two different approaches to road traffic modeling. The first one, called macroscopic, describes the traffic as a whole in terms of physical quantities such as traffic flow and traffic density. The state of such models is changed based on differential (or, in the case of computerized models, difference) equations describing fluid dynamics. The second approach, called microscopic, describes the traffic at a greater level of detail, namely in terms of individual traffic participants (e.g., cars, trucks, streetcars, or even pedestrians). The state of such models is changed based on complex algorithms describing the state variables (e.g., position, speed, or acceleration) of each traffic participant. More details can be found, for example, in (Hämäläinen, 2006).

Regardless of which approach is used, there is an aspect that all traffic models have in common. It is the underlying streets and intersections, called a traffic network in short. In multiadjustable road traffic models, the traffic network is composed of a set of interconnected structural components. Originally, we defined a structural component as either an intersection or a road segment connecting two intersections, but smaller parts of traffic network can also be considered structural components at the points where the number of traffic lanes changes (see Figure 1). Similarly, modeling individual traffic lanes by separate structural components can also be helpful under certain conditions.

In order to enable multiple-level-of-details modeling, the overall model needs to be subdivided into several areas, each modeled at either macroscopic or microscopic level of detail. For this purpose, structural components are a good choice, because they can easily provide different granularity of this subdivision. So, each structural component shall be looked upon as a standalone submodel of a specific small area.

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Figure 1: Example of decomposing a part of a traffic network into structural components (bounded by dashed lines). In this case, any change in number of traffic lanes constitutes a structural components boundary.

This also means that we need to distinguish between macroscopic and microscopic structural components, because their modes of operation are different. Macroscopic structural components obtain the values of the physical quantities describing the traffic dynamics from their neighbors, compute new values of these quantities based on the corresponding difference equations, and pass these new values to the neighbors again. Their behavior is therefore rather simple and constant. On the other hand, the behavior of microscopic structural components is much more complex. They need to accept traffic participants coming from structural components adjacent to them, then to pass these traffic participants along their topology using some complex algorithms and finally to pass them to some other adjacent structural Their behavior is composed of many components. submodels (e.g., car-following model or lane-changing model), so they can make use of behavioral components in order to make their behavior adjustable to the conditions being modeled, such as local traffic law. For more details about behavioral components, see (Zelenka, 2009).

Because macroscopic and microscopic structural components communicate in different terms (physical quantities vs. traffic participants), they cannot be interconnected directly. Instead, adapters (i.e., intermediate components that serve as interpreters) must be placed between them. In the direction from a microscopic to a macroscopic component, the adapter needs to obtain the values of the respective quantities using statistical analysis, in the opposite direction, it needs to generate the traffic participants according to the values of these quantities.

The preceding paragraphs imply that structural components are the active elements of the simulation. That is, they are responsible for updating the state and position of the traffic participants. This is a big difference compared to most existing microscopic road traffic simulation tools, where the traffic participants update their state and position themselves. However, making the structural components active has some additional advantages. For example, consider the situation from Figure 2. There are four cars situated at an uncontrolled intersection. At uncontrolled intersections, cars are required to give right of way to the cars approaching from the right side in most countries. Consequently, each of these cars is required to give right of way, effectively causing a deadlock. To resolve this situations, the drivers need to agree on who will travel through the intersection first. When the cars are the active elements, it is not easy to detect this situation, nor it is to resolve it. In fact, it requires some distributed algorithms to be implemented within the model. When we make the structural components to care for updating car states and positions, detecting and resolving this situation is easy, because there is only one element (the structural component) responsible for doing it.



Figure 2: A deadlock situation caused by four cars situated at an uncontrolled intersection.

Moreover, even if the cars were the active elements, some structural components would also have to implement some behavior. An example can be traffic-light operated intersections, which need to implement some logic determining which traffic participants are allowed to travel through it at which times.

DESCRIBING AND GENERATING THE TOPOLOGY OF STRUCTURAL COMPONENTS

Most of the existing microscopic road traffic models are based on cellular automata. According to (Chopard and Droz, 1998), a cellular automaton is a lattice of cells in *d*-dimensional space, where each cell is associated with a Boolean flag representing the state of the cell (i.e., empty or occupied), supplemented by a rule (same for all the cells) describing the time evolution of these states. In the case of road traffic models, d = 2 and the state-changing rule is represented by the complex behavioral model mentioned in the preceding section. One of the most well-known (and still very popular, especially for its simplicity) road traffic models based on cellular automata is the Nagel-Schreckenberg model; see (Nagel and Schreckenberg, 1992).

For cellular-automata-based microscopic models, the topology of structural components will be composed of individual cells. Unfortunately, macroscopic structural components are spatially compact. This difference is somewhat unpleasant, because it means that we either need to maintain two separate descriptions of the traffic network or need to find a description that can be used for both macroscopic and microscopic models. Further, from our previous experience we know that storing information about a traffic network at the microscopic level of detail shall be avoided, because it constitutes a serious performance bottleneck at simulation startup when an enormous amount of data needs to be loaded from some slow external memory. To overcome these two issues, we need to find a minimum set of information that unambiguously describes the traffic network and from which the rest of information (e.g., the positions of the individual cells) can be generated.

In general, there are two basic requirements that the topology of structural components shall satisfy. The first one is that lengths are reproduced to some scale. Satisfying this requirement is essential, because any disproportion between lengths in the model and lengths in the real situation inevitably means an error in results of the simulation. The second one is that the overall topology of the traffic network in the model resembles its real counterpart as closely as possible. This requirement is in fact completely unnecessary for the correctness of the model, but is important for proper visualization of the simulation results. Since a long time ago, people have been accustomed to visualize geospatial information in the form of maps. So providing the results of the simulation in a map-like user interface makes them easier to understand than, for example, writing them as an obscure matrix of numbers.

There are two aspects in describing the topology of a structural component. The first one is the general topology (i.e., the shape and dimensions) and the position in space. In this case, we can follow geographic information systems, which also deal with this aspect. The second one, specific to the domain of cellular-automatabased simulation models, is the layout of the cells inside this general topology.

Describing Traffic Lanes and Road Segments

Let's look at the structural components in greater detail. The most simple structural component to think about is



Figure 3: An example of reducing the representation to a guideline and further to a sequence of control points (C_1, C_2, C_3, C_4) through which it passes (top). An example of generating cells along the guideline (bottom).

probably a traffic lane. Any road segment can be composed of one or more traffic lanes. One traffic lane constitutes an one-way road. Where more traffic lanes are present within a road segment, the road can be either an one-way road (all traffic lanes oriented in the same direction) or a two-way road (some of the traffic lanes oriented in one direction, some in the opposite one). Describing the general topology of a single traffic lane is actually quite easy. If we assume that the traffic lane has a constant width (most often, the minimum width defined by some construction standard is used in real situations), we can reduce the description to a single curve (see Figure 3, top). Further, we can represent a curve by a set of points through which it passes, because the original curve can be regained by interpolating them. If we had many points, we could simply connect them by straight lines. In our case, when we are trying to find a minimum set of these points, we more likely want to use some interpolating curve. As a conclusion, traffic lanes can be described by a set of node points.

Describing Intersections

With intersections, the situation is more complicated. The general topology of an intersection can be derived from the traffic lanes that are connected by the intersection or, to be more precise, their corresponding end points. In fact, the tangential vectors to the traffic lanes in these end points are also needed (see Figure 4), but they can be easily calculated using the waypoints adjacent to the end points. Therefore, the minimum set of information to describe the general topology of an intersection is the set of end points of the adjacent traffic lanes. However, to generate the cells within the intersection, some additional information is necessary.


Figure 4: An example of representing an intersection by the end points of the adjacent road segments and the tangential vectors to these road segments in their end points.

We need to know which pairs of traffic lanes shall be interconnected (i.e., to which outgoing traffic lanes it is possible to travel from each ingoing traffic lane). Based on this information, we can generate a guideline representing the trajectory through the intersection for each such pair. We have studied the trajectories of vehicles traveling through intersections and we came to a conclusion that these trajectories are best represented by rational Bézier curves.

A rational Bézier curve is a special Bézier curve that assigns each control point an adjustable weight in order to become a closer approximation to an arbitrary shape. A rational Bézier curve of degree n (i.e., defined by n + 1control points) can be expressed by Equation (1), where P_i is the *i*-th control point, w_i is its weight, and the parameter t takes the values from 0 to 1.

$$Q(t) = \frac{\sum_{i=0}^{n} \binom{n}{i} t^{i} (1-t)^{n-i} P_{i} w_{i}}{\sum_{i=0}^{n} \binom{n}{i} t^{i} (1-t)^{n-i} w_{i}}$$
(1)

For our purpose, a rational Bézier curve of degree 2 is appropriate. The control points (see Figure 5, top) are the two end points of the interconnected road segments (S, E) and either the point lying in the middle of the straight line connecting these two end points (if they are collinear) or the intersection point (C) of the tangential vectors to the interconnected road segments (in all other cases). The weights w_i are equal to 1.0 in points S and E and greater than 1 in point C. In our experiments, a value around 2.5 provided the most realistic trajectory.

Generating Individual Cells

So far, we dealt with the general topology of structural components. But, as mentioned above, we also need



Figure 5: An example of a trajectory through an intersection defined by a rational Bézier curve (top). An example of overlapping cells generated on different guidelines (bottom).

to deal with the other aspect of the structural components, that is generating the individual cells. In most cellular-automata-based road traffic models, circular cells are used. The center of each cell shall lie on a trajectory which the traffic participants follow, so we can use the above-described curves as guidelines for the cell generation (see Figure 3, top vs. bottom). The diameter of cells then uniquely defines the number of cells that are to be generated on a guideline with a certain length. In practice, these diameters differ from model to model. The reason is that their value, in connection with the length of the time step in which the state of the model is updated, determines the possible discrete values of speed that is possible to model. Most often, diameters range from 2 to 3 meters.

Although the centers of the individual cells are uniquely defined by the length of the guideline and the diameter of the cells, it is not so straightforward to calculate them. The first problem is that the length of the guideline needs to be determined. For most curves, there is unfortunately no formula to return the length of it. And, even if there is one, it requires the curve to be defined analytically, because it usually involves integration. So, we need to use another approach. For curves that are defined using a parameter, it is possible to generate points lying on the curve by substituting in some increasing values for the parameter and then to approximate the curve by a polyline (i.e., a set of straight lines connecting adjacent points). This is sometimes called tessellation of the curve. Calculating the length of a polyline is easy, so the main concern is to find an reasonable number of points to use, because too few points means an inaccurate approximation and too many points means an unnecessary computational overhead. The second problem is that the tessellation needs to be equidistant so that the cells fill the space uniformly. This may seem easy at first glance, but most curves (rational Bézier curves not being an exception) cannot be tessellated equidistantly by increasing their parameter by a constant step. Instead, a technique called reparametrization by arc length needs to be used; see (Schneider and Eberly, 2002, p. 890). Reparametrization by arc length is based on solving Equation (2) for some value x, where Q(x) is a point on the curve for parameter value x, Q(S) is the starting point of the curve, and L is the desired length from this starting point.

$$Q(x) - Q(S) = L \tag{2}$$

Typically, Newton's method is used, but this also causes an unnecessary computational overhead. In our case, performing the tessellation for some smaller parameter step and saving the resulting points together with their distance from the starting point of the curve into a search table seems to be a better solution, as it allows us later to use the nearest point from this table.

Now, we are able to generate the cells. However, there is still one problem to be solved. In intersections, there are guidelines that either intersect in some point or are leading close to each other in some area. Consequently, generating the cells on these guidelines leads to cells that overlap (see Figure 5, bottom). This means that, in the real world, there is not enough space for two cars to fit in the area modeled by these cells. There are basically two different solutions. The first one is to replace these cells by a single one (its center could be the midpoint of the line joining the centers of the replaced cells, for example). This would decrease the number of cells in the model, but would also cause unrealistic deviations in car motions during visualization. The second solution is to use a single state (see the Chopard and Droz definition of a cellular automaton above) for all the overlapping cells (i.e., to mutually exclude the cars from entering the area).

Referencing to a Particular Position in a Traffic Lane

Finally, we need to provide a means for associating additional information with parts of the traffic network. Examples of such information may be speed restriction or reserving a traffic lane for some particular traffic only. Because this information can begin and end somewhere inside the structural components, we need to associate it with the individual cells to which it relates. This means that we need to reference cells which do not exist yet. We can describe the additional information by its type and its impact point (i.e., a point where its validity begins or ends). The impact point can be determined using the distance from the starting point of the guideline associated with the structural component (see Figure 6). Based on this information, the cell to which this point belongs can be determined.



Figure 6: An example of referencing to an impact point based on lengths. Here, the impact point is located in l/L of the structural component.

RESULTS

The vehicle trajectories represented by a polyline generated using rational Bézier curves (weights in end points $w_{0,2} = 1.0$, weight in the middle control point $w_1 = 2.5$) and the equidistantly distributed cells generated along this trajectories are presented in Figures 7 to 10. It can be seen that the shapes of the trajectories clearly resemble the shapes of trajectories of vehicles driving through a smooth bend. The figures showing overlapping cells can seem confused at first sight, but it should be kept in mind that the cells only serve the purpose of computing the simulation state and are typically not visualized in any way. Conversely, their placement along the smooth vehicle trajectories make the visualization of cars traveling through an intersection more natural and therefore pleasurable.

SUMMARY

In this paper, we dealt with structural components in multiadjustable road traffic models. In the first part, we presented some reasons for making them the active part of the model and showed that it has more advantages than just enabling multiple-level-of-detail modeling. In the second part, we investigated the possibility of finding a single description of their topology suitable for both macroscopic and microscopic modeling. We



Figure 7: An example of a trajectory through an intersection defined by a rational Bézier curve (top). An example of cells generated along this trajectory (bottom).

identified a minimum set of information that is necessary to describe a traffic network and provided some methods for deriving the rest of information from this minimum set.

The experience gained from this research and the previous research of behavioral components will be used to develop an experimental multiadjustable road traffic model. Together with the experience from (Hájková, 2005), it will be also used to support this experimental model in the areas of preparing the maps of traffic networks and visualizing the simulation results.

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Figure 8: An example of trajectories through a Y-shaped intersection (top). An example of overlapping cells generated along these trajectories (bottom).

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Figure 9: An example of trajectories through an X-shaped intersection (top; some trajectories have been omitted for the sake of clarity). An example of overlapping cells generated along these trajectories (bottom).

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Figure 10: An example of trajectories through an irregularly shaped intersection (top; some trajectories have been omitted for the sake of clarity). An example of overlapping cells generated along these trajectories (bottom).

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RESTRUCTURING OF AN ORDER PICKING SYSTEM FOR A MAIL ORDER COMPANY

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KEYWORDS

order-picking systems, rough planning, simulation modules, dimensioning, decision making, logistics, material flow, PlantSimulation

ABSTRACT

Planning a new logistics center is a quite difficult job. Depending on the requirements there are a great number of possible design versions. The planner has to consider not only the present but also the future requirements. Up to now, the planner decides on the basis of experience which system will perform the requested services best. This paper illustrates the redesign of a new order-picking system in industry supported by a simulation tool of our institute designed especially for the rough planning. With the described project the road capability of the applied simulation concept is underlined. Several versions based on the requirements were investigated and evaluated. Key figures are calculated and a recommendation depending on performance and arising expenses is given.

INTRODUCTION

Are order picking systems plannable? Is it not rather a gamble that the future requirements of a picking system are interpreted correctly? In many cases it can be observed that the planned capacity of a new system is already insufficient at the start of operation. Thus, for instance, a high bay warehouse of the company Würth in Bad Mergentheim had to double capacity eight months after the start of its operation. Was it a planning error? [Vollmers 2007]

The dilemma during the planning process of picking systems is the sum of changing factors such as the assortment, the order structure, functions and other unexpected changes. [Dörrie 2007] The variety of design options for these systems complicates the selection of an appropriate technology [Dullinger 2005]. To reduce the risk of planning errors the planning has to be fulfilled for a time horizon instead for a single point in time. [Günthner 2008]

By using scenario analysis for the extrapolation of requirement data the risk for estimating future

requirements can be reduced. This can be achieved by changing different influencing factors and setting them into relation. In combination with a modular and scalable design of the picking system the planning dilemma can be resolved.

For the support of the planning process the Institute for Materials Handling, Material Flow and Logistics developed a planning software. In addition to the data analysis and extrapolation, creation of simulation models in PlantSimulation can be done quickly by the software. Thus, it is possible to use simulation during the phase of rough planning of picking systems. [Ulbrich 2007]

Meanwhile the planning software is assembled for real planning projects. In this paper a practical example of an online trade will be discussed in depth.

The company has operated a rapidly growing online shop for wholefood products and gluten-free foods for about four years. To meet the increasing cost pressure and master the highly competitive market the company moves to a new logistics center.

With this move the company expects reduced logistics costs and increased capacity for the growth target.

REQUIREMENTS

The current process was analyzed by methods time measurement (MTM) during several local appointments in the old logistic centre. With help of the deployed Warehouse Management System (WMS), the current order and assortment structure was reviewed. The actual assortment includes 3.042 articles and the structure of access frequency follows the classical Pareto-distribution. Today, the company forwards about 1.500 orders per day. An average order consists of four lines with a quantity of 1,5 items.

Table 1: expected growth of essential key data

expected	Scenario	Scenario	Scenario
growth per year	positive A	positive B	constant
assortment	8 %	4 %	0 %
orders	10 %	5 %	0 %

During a one-day workshop together with the employees of the company the requirements of a new

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logistics centre were defined. The essential key data are illustrated in **table 1**.

By using the above-mentioned planning software during the workshop the estimation of growth, e.g. three percent more articles p.a., was easily adjusted by pictured diagrams.

PLANNING VERSIONS AND MODELLING

The maximum dimensions of the picking system were already given because the leasing contract of the building which is designed to be the new logistic centre was already concluded. Due to the rapid changes in market segment of online trading the company has excluded extensive investments in automation. Therefore the new picking system should be based on the classical principle of person to goods.

Several planning versions were prepared by the Institute for Materials Handling, Material Flow and Logistics (Technische Universität München) and these versions were aligned with the company in a second workshop. In all versions shelved rackings were intended for the picking area. Differences between them are distinct locations of the main lane and the base. For the investigation the following variants were selected:

- The main lane is in front of the lanes called head lane (type 1a)
- Head lane and one shortcut between the lanes (type 1b)
- Head lane and two shortcuts between the lanes (type 1c)
- Head lane and maximum (five) shortcuts between the lanes (type 1d)
- The main lane across the picking area, called central lane and the base is located in front of the picking area, called border base (type 2a)
- Central lane, border base and one shortcut (type 2b)
- Central lane, border base and two shortcuts (type 2c)
- Central lane, border base and maximum (three) shortcuts (type 2d)
- Central lane and the base is located in the middle of the picking area, called central base (type 3a)
- Central lane, central base and one shortcut (type 3b)
- Central lane, central base and two shortcuts (type 3c)
- Central lane, central base and maximum (three) shortcuts (type 3d)

Figure 1 illustrates four of the abovementioned versions.



Figure 1: layout of selected planning versions

In addition to the layout versions several process versions were analyzed and worked out. An important question was, how many orders should be handled by the picker on a collective round tour through the picking area. Picking more than one order by a person at the same time is called multipicking. The advantage is that the picking density is higher by using multipicking than collecting only single orders at the same time. Because of the average article weight and volume it was determined that a maximum of six orders can be processed by a single collective round tour.

One of the next questions was which path strategy should be used for picking? In a preliminary investigation different picking strategies such as the classical picking, serpentine picking or largest gap picking strategy were thoroughly discussed. Depending on the path strategy for picking a compatible storage strategy for articles in the picking area had to be selected. The preliminary investigation reasoned that depending on this article structure the branch aisle strategy with a concentration of fast movers around the base is advantageous and recommended [Roodbergen 2008, Petersen 2004, ten Hompel 2007].

These strategies are used for all versions, thus the number of simulation test runs can be bounded. In the following morphological box the analyzed influencing variables are illustrated. For the analysis 1.620 simulation test runs were performed. A simulation test run needs approximately three minutes of computing time.

	ana	lysis			
layout position of main lane	in front of picking area (head lane) In the middle of picking area (central lane)				
position of base	borde	er	center		
shortcuts	none	one	two	max	
		12 layou	it versions		
organisation					
multipick	none 3 or		rders	6 orders	
	3 organisation types per layout version				
load scenarios					
scenarios	positive A	posi	tive B	constant	
periods / years	2009	2010 12 load	2011 scenarios	2012	
simulation runs		2 2.160 sim	3 ulation run	4 5 s	

Figure 2: Combinations of layout, organization and load version for analysis

The processes which were developed within the second workshop, were described by means of MTM which is aided by the planning software. The outcome of this are determinated times describing various process steps, e.g. the grasp at a single item. These times are provided for the simulation model.

The entire planning software environment uses a relational data base on the bottom layer of its architecture. In the database all information needed for simulation are saved during the planning steps and the several versions of the picking system are described in a formal structure with the aid of the planning software. This description includes the layout, the processes and the load scenarios. Simulation models in PlantSimulation can be generated completely and automatically by the information saved in the database. One of these generated models can be viewed in figure 3.



Figure 3: Generated model for type 3b compared with the layout

The automatical generation of simulation models become possible through the definition of standard elements which are strung together according to the values of the parameters set in the database by the planner.

RESULTS AND INTERPRETATION OF SIMULATION OUTPUTS

Consecutively the results for the average time per order line in minutes simulated by PlantSimulation are illustrated in **table 2**.

Table 2: average time per order line in seconds for the	e
load scenario "positive A & 2009"	
(average over five simulation test runs)	

	number of orders per tour				
	one	three	six		
Head lane (type 1a)	21,60	13,20	9,84		
Head lane and one	19,80	12,60	9,90		
shortcut (type 1b)					
Head lane and two	18,82	12,61	10,05		
shortcuts (type 1c)					
Head lane and	18,86	12,63	10,90		
maximum (five)					
shortcuts (type 1d)					
Central lane and	19,80	12,00	9,18		
border base (type 2a)					
Central lane, border	19,75	12,20	9,66		
base and one shortcut					
(type 2b)					
Central lane, border	19,78	12,21	9,84		
base and two shortcuts					
(type 2c)					
Central lane, border	19,80	12,22	10,38		
base and maximum					
(three) shortcuts (type					
2d)					
Central lane and center	18,00	11,40	8,88		
base (type 3a)					
Central lane, center	18,10	11,70	9,24		
base and one shortcut					
(type 3b)					
Central lane, center	18,25	11,72	9,50		
base and two shortcuts					
(type 3c)					
Central lane, center	18,30	11,73	10,00		
base and maximum					
(three) shortcuts (type					
3c)					

In figure 4 the various layout versions are shown with the calculated seconds per orderline.



Figure 4: seconds per order line by six orders per tour

As illustrated in figure 4 with the circle marked point, the best version depending on the seconds per orderline is type 3a. This is caused by the central location of the base which reduces the time units for changing lanes. One of the main disadvantages is the transport of the bins from the base to the shipping area. Because our client required a continous flow of the bins the need for material handling between base and shipping area was indispensable. Although this could be solved through a material handling for level changing the investment increases so that version type 3 is too expensive in comparison with the other versions. The outcome of this is the necessity for the calculation of the investment and arising expenses before the best version can be identified. This will be done in the next step.

VERSIONS BENCHMARK

The analysis of simulation results is the first step for the evaluation of planning versions. Besides the comparison of different versions by performance, the results of simulation together with the formal description of the picking systems provide the basis for the monetary evaluation.

If a rough calculation of investment and operational costs is sufficient for the comparison of versions, the planning software can be used. Therefore several cost rates are defined in the database. With the information from the formal description and the cost rates the software can calculate the rough investments value. The operational costs as depreciation and maintenance costs for instance derive from the calculated investment. The approach is shown in. figure 5.



Figure 5: approach to calculate the investment and costs

Personnel costs were defined in agreement with the company. Therefore the demand of staff is identified and described depending on the system load. Based on this demand, the number of appointed employees is fixed under consideration of absent and sick days.

Preparing decision-making some important monetary key figures are calculated to benchmark the different planning versions. The main key figures are the performance in time per orderline, the costs per orderline and the costs concerning an order. The values are illustrated in figure 4 and figure 6 for some selected versions.



Figure 6: cost comparison between selected versions

Best performance is reached by the versions of type 3 but the transport of bins from the center of the picking area is complex and requires a larger investment because a level change is necessary (vertical conveyer needed). Considering the monetary benchmark the versions of type 2 and 1 are more profitable. This is a typical result which can be compared with the studies of Schulte [Schulte 2003].

Additionally, the future fulfillment of requirements had to be considered in the evaluation of the planning versions. The trend of the cost structure over the life cycle of a system has to be considered in the benchmark. Figure 7 shows the cost per order over the planning horizon depending on the different load scenarios for version type 2a.



Figure 7: cost schedule for planning version type 2a

With these key figures, the planning versions can be compared quickly. In addition, an efficiency analysis was performed in agreement with the employees of the company. Some of the central concerns were the process safety and ergonomics.

Based on all the above-mentioned information the company could choose one of the planning versions, which will lastly lead to the detailed planning.

Finally the central lane with the base at the border was selected justified by the best cost structure and expansion options.

CONCLUSION

First, the order picking then the stock planning – In the order picking area usually the most staff is employed whereby the customer service and the logistics quality are decided. The highest costs are incurred in this area. [Gudehus 2006] The planning of an order picking system is characterized by the complexity of the system, due to the many interactions between the influencing factors and the multitude of design options. The simulation is the appropriate tool to investigate these interactions.

In the phase of rough planning a large number of versions have to be examined, so that the creation of simulation models has to be mandatory fast. The planning software and the simulation modules with its parameters in PlantSimulation offer this opportunity. Thus, an efficient use of simulation in rough planning becomes possible.

With the aid of consolidated results from rough planning, the company has created a set of specifications. Currently the tender is running and the implementation is scheduled for spring 2009, so that the new logistics center can be obtained in the slack summer months.

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SIMULATION STUDY OF THE SHORT BARREL OF THE GUN MANUFACTURE

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KEYWORDS

Discrete event systems modelling and simulation, simulation of manufacturing, Witness.

ABSTRACT

This paper deals with the use of computer simulation aiming at more efficient production of the manufacturing system. In our case, the possibilities of use are demonstrated on a particular example from industrial practice. The purpose was to build up a model of the existing short barrel of the gun manufacturing line, and, especially, to propose a solution for increase of productivity, and to find bottlenecks of the system. The Witness simulation environment was used for modelling and subsequent simulation. On the basis of predefined requirements of the user, several simulation experiments were suggested. The results of these experiments have revealed non-economy and a very small passage ability of the existing system.

INTRODUCTION

The computer simulation of discrete events is becoming a necessary supporting instrument in making the operation of production systems more effective. Among other things, this is due to its capability of simulating and following up both stochastic and dynamic properties of individual processes, and thus predicting their behaviour.

In the present so-called turbulent environment, any effective operation of the production systems cannot be achieved any more only by local optimization of individual parameters or subsystems. These are so interacting that it is not possible to solve them separately, and the whole system has to be considered globally, and the optimum of the system as a whole must be searched for. High dynamics, complexity and, as such, also insecurity at the solution of company tasks require more and more the use of such methods and such supporting means that allow a complex access to the design of production systems, as well as fast tests of a variety of different variants of the solution, and thus minimization of a risk of erroneous decisions. Therefore, a significant help is a complex dynamic analysis of the production systems by means of computer simulation. So, at the present time, the computer simulation is a necessary part of every large production process. With its help you can perform the simulation of real environment. If the process has been modelled correctly, the production simulation can be made for a few days or weeks in advance. This instrument gives the companies the possibility of operational planning at minimizing energies, inventories and labour.

This paper deals with the simulation study of a particular manufacturing line, in our case this is the short barrel of the gun manufacturing line in a company producing the guns. The production process is described in detail in Section 2. This study includes an analysis of the current status of the plant, data collection, construction and verification of the model, and, in particular, a proposal and implementation of simulation experiments. The aim was to propose a solution for increase of productivity and to find bottlenecks of the manufacturing system. The simulation experiments were proposed on the basis of the predefined requirements of the user. The task was to determine an appropriate number of machines in individual workplaces, or, rather, to establish a correspondent number of shifts of the operation of these workplaces. The Witness simulation environment was used for the construction of the model and subsequent simulation. Basic information on this environment is to be found in Section 3. In this Section, the process of model creation in the Witness environment is outlined. Description of the proposed simulation experiments and evaluation of achieved results is presented in Section 4.

DESCRIPTION OF THE SHORT BARREL OF THE GUN MANUFACTURE

The machines used in the manufacture serve for machining the products in various production phases. These are, in particular, lathes, grinding and drilling machines. All these machines are machining only one product at a given moment. Thus, only one part enters the machine and a specific operation is carried out on it, and also only one part leaves the machine. Individual machines are arranged into groups. Each group forms a workplace to perform a certain operation. Every machine (except for one machine) is operated by one operator. For this reason, labour does not have to be considered in the model. Table 1 shows quantities of machines in individual workplaces which are used in the system for machining the products, together with the number of shifts during which the workplace is in operation.

Table 1: Number of machines in individual workplaces
and number of shifts

Workplace	Description of workplace	Number of	Number
No.		machines	of shifts
1	Drilling of the short		
	barrel of the gun	3	2
2	Drilling -countersinking	1	2
3	Turning-Lathe – Fischer	3	2
4	Turning-Lathe - SV 18	7	2
5	Turning-Lathe - Liberty	6	2
6	Honing	5	2
7	Forging	2	3
8	Grinding	6	2
9	Turning-Lathe –		
	chambers	3	2
10	Polishing - chambers	2	2
11	Manual treatment	9	1

Each workplace performs a certain operation. The product comes through some workplaces repeatedly, therefore one workplace carries out a few different operations. The manufacturing process is described step by step below, in Table. 3. Here is given the number of the workplace where a particular operation is made, and the time of individual operations. This data was provided by the operator of the plant from its planning system where the data for all machines are stored. The data collection was carried out in that workplace for a long time, hence we can consider this data to be very correct. So any further measurement directly in operation would be just waste of time.

Products' handling in the production is made with the help of vehicles. Material handling is not controlled in real manufacture; this is done in case of emptying individual buffers. Time of material handling from one machine to another is minimal, as the distance is very short. Therefore we can say that the time of material handling is negligible.

The manufacturing plant works in three-shift operation. Most workplaces are in two-shift operation, though (see Table 1). Overview of individual working shifts of the manufacturing system is shown in Tab. 2.

Table 2: Working shifts of the department of shortbarrel of the gun

Shift	Shift	Break	Shift
	start		end
Morning shift	5:45	10:30-11:00	14:15
Afternoon shift	14:00	17:30-18:00	22:00
Night shift	22:00	2:00-2:30	6:00

In operation, maintenance of the machine is done on a regular basis. Thanks to this maintenance, faults occur on individual machines only exceptionally. Time of maintenance together with elimination of faults will take 3 % of machine time.

Table 3: Manufacturing procedure of	of the short barrel of
the gun	

Operation	Description of operation	Workplace	Process
1.	Hole drilling for preparation of a	1	17,4
	bore		
2.	Countersink of ends at the bored hole	2	7,8
3.	Turning of the recess on one side of	3	14,4
	the cut for clamping onto the copying machine		
4.	Turning of surface either for cone or	4	13,8
	cylinder shape according to the type		
	of the forging, or final shape of the		
5	short barrel of the gun, respectively	5	10.2
Э.	Execution of ends is done for	3	10,2
	operations that follow		
6	Honing This is final treatment of the	6	40.2
0.	hole before the very forging.	Ŭ	10,2
	Honing is done to achieve necessary		
	hole size and roughness		
7.	Forging is carrying out the final	7	49,2
	sizes of the bore and surface of the		
	forged piece as per the calibre		
	required and type of the short barrel		
0	of the gun	4	10.2
δ.	Cutting-off and planing the face of the short harrel of the gup to the	4	10,2
	length required acc. to the type – the		
	so-called first face		
9.	Turning operation of turning of the	3	22.8
	faces and recess		,
10.	Again, cutting off, countersinking,	4	155,4
	milling of the shape in the area of		
	the cartridge chamber, turning of the		
	diameter of the short barrel of the		
1.1	gun plus addition under the grinder	0	01.0
11.	Grinding of the diameter of the	8	94,8
	size shape and machining		
12	Turning with connection to the	5	84
12.	subtoothing and the very turning of	5	57
	the toothing		
13.	Turning of the cartridge chamber	9	91,2
	and turning of the muzzle, where its		-
	final length is determined acc. to		
	individual types		
14.	Polishing the chute and polishing the	10	28,2
	cartridge chamber		1.2
15.	Checking and preparatory activities	11	1,8
	for the next work with the product,		
	conservation coat degreesing etc		
	conservation cout, degreasing, etc.	1	

The simplified scheme of the operation of the production plant is presented in Figure 1.



Figure 1: Simplified scheme of the operation of the production plant

MODEL CONSTRUCTION IN WITNESS SIMULATION ENVIRONMENT

For building up the model and subsequent implementation of the proposed experiments, it is possible to use a wide range of simulation programs and systems (Banks 2005). The Witness system environment was available in this case. This system is offered by the Lanner Group and it contains many elements for discrete-part manufacturing. Witness models are based on template elements. These may be customized and combined into module elements and templates for reuse. The standard machine elements can be single, batch, production, assembly, multistation or multicycle. Other discrete modelling elements include multiple types of conveyor, tracks, vehicles, labor and carriers. The behavior of each element is described on a tabbed detail form in the Witness user interface. The models are displayed in a 2-D layout animation with multiple windows and display layers.

Every operating workplace of the manufacturing line is modelled in the Witness environment with help of the element Machine of Single type. Parameters of each element are set by means of tabbed detail form. Quantity of machines in the particular workplace and cycle time are set up according to Table 1 and Table 2. If a workplace carries out a few operations with a different cycle time, this parameter is considered as a variable. The value of this variable is then set up in the output rule of the buffer in front of the workplace concerned.

Products' handling in the manufacture is performed by vehicles. These are modelled with help of the element Vehicle. These vehicles move along the predefined tracks (modelled by means of the element Track). In the simulation model, the handling is carried out at the moment when quantity of products in the buffer has decreased under a value of 3. Capacity of each buffer is 5000. As mentioned above, time of material handling from one machine to another is minimal.

For creating the model of process of maintenance and fault in individual workplaces, an auxiliary element of Machine type is used, which takes care of fault generation (maintenance on individual machines of the particular workplace). Thus, each workplace has its fault generator. This solution is given by the fact that it is not possible to set up a fault only on one machine of the particular workplace which is just modelled by the only element. A fault (or maintenance, respectively) is generated by means of a new part (element of Part type), which at the input into the particular fault generator will cause a fault on the corresponding machine of that workplace. Time of fault (maintenance) is set up by means of the parameter Cycle Time of the fault generator. For generating a fault (maintenance), normal distribution is used. The parameters are chosen so that a fault (maintenance) occurs on each machine at least once a day.

In the model, working shifts are made with help of the element Shift. For purposes of the simulation, three one-week shifts were created on the basis of Table 2. The shifts were then assigned to the individual workplaces as per the number of shifts in which the particular workplace is in operation every day.

SIMULATION EXPERIMENTS AND RESULTS

After building up the model of the manufacturing line, the proposed model must be first verified. The verified model will be subsequently used for simulation experiments. As the system in view works in continuous operation, the model would have to be first filled with products in order to verify the model with the real system. This can be made in the Witness environment due to the parameter WarmUp Period. The value of this parameter determines the time when the followed-up statistics and variables are zeroized. The value WarmUp Period is set up to 172800 seconds, which corresponds to the time of 2 days. This time is sufficient for filling the whole model with products. Total time of simulation is 2 weeks (that means 2 days Warm Up, 12 days testing period). The Tables given below show the results of individual simulation experiments.

Simulation of the current status and verification of the model

One of the most important and difficult tasks facing a model developer is the verification and validation of the simulation model. There is a great number of verification, validation and testing techniques. It is possible to classify these techniques into four primary categories: informal, static, dynamic and formal (Banks 1998). From the point of view of this terminology, only informal and static techniques were used. During the verification, especially percentage capacity utilization of individual workplaces and total production of the manufacturing line were monitored (see Table 4). The values of monitored characteristics are comparable to those of the real system. The Table 4 shows ineffective operation of this manufacturing system. More than half of workplaces are blocked. It is caused due to filling the buffers between individual workplaces (capacity of buffers is 5000). Busy time of most workplaces is less than 50%. Workplace of Honing is the critical point of system (busy time practically 100%, 3% maintenance).

Proposal of model parameters changes resulting in increase in production efficiency

The simulation experiments were suggested on the basis of the predefined requirements of the user:

- It is possible to reduce the number of machines in individual workplaces
- It is not possible to increase the number of machines in a workplace
- It is possible to change the number of working shifts of individual workplaces

The task was thus to determine an adequate number of machines in individual workplaces, or possibly, to set up an appropriate number of working shifts of the operation of these workplaces.

Numbers of modifications were gradually proposed for the present status of the manufacturing line. All the proposed experiments were simulated. Description and results of some experiments are presented below.

Report on individual workplaces					
Workplace No.	Description of workplace	Number of machines	Number of shifts	Busy Time [%]	Blocked Time [%]
1	Drilling	3	2	35,10	61,87
2	Countersinking	1	2	46,73	50,13
3	Turning-Lathe – Fischer	3	2	34,94	60,39
4	Turning-Lathe - SV 18	7	2	43,58	53,43
5	Turning-Lathe - Liberty	6	2	30,15	57,14
6	Honing	2	2	96,95	0,00
7	Forging	2	3	66,38	16,74
8	Grinding	6	2	23,00	0,00
9	Turning-Lathe – chambers	3	2	47,49	0,00
10	Polishing - chambers	2	2	22,02	0,00
11	Manual treatment	9	1	0,54	0,00
TOTAL 44 22 40,63				40,63	27,25
Number of necessary labour per day			8	31	
Total production of manufacture [pieces]					230

Tab 4: Report on results of current manufacturing line

Experiment No.1

Experiment No.1 eliminates the significant bottleneck of current manufacturing system by means of increasing the number of working shifts. Operation time of workplace Honing was set to three shift operation. Due to high manufacturing capacity of machines before workplace Honing and inadequate capacity of Honing many workplaces became blocked. Blocked Time of these workplaces can be reduced with cut in manufacturing capacity of workplaces Drilling and Countersinking. Further the unsuitable number of working place of Manual treatment is reduced. Results of this simulation experiment are shown in Table 5. Proposed changes are highlighted. Original values are stated in the brackets.

More than double Total production increase and labour cuts (11 labourers) are reached in this experiment. Disadvantage of this experiment consists in partial blocking the Turning-Lathes - Fischer resulting from maximum busy time of Turning-Lathes - SV18. The experiment No.2 solves this problem.

Report on individual workplaces					
Workplace No.	Description of workplace	Number of machines	Number of shifts	Busy Time [%]	Blocked Time [%]
1	Drilling	2 (3)	1 (2)	96,99	0,00
2	Countersinking	1	1 (2)	86,95	0,00
3	Turning-Lathe – Fischer	3	2	60,04	18,41
4	Turning-Lathe - SV 18	7	2	97,01	0,00
5	Turning-Lathe - Liberty	6	2	59,03	0,00
6	Honing	2	3 (2)	73,17	0,00
7	Forging	2	3	90,85	0,00
8	Grinding	6	2	56,69	0,00
9	Turning-Lathe – chambers	3	2	97,03	0,00
10	Polishing - chambers	2	2	45,01	0,00
11	Manual treatment	1 (9)	1	10,95	0,00
TOTAL 35 (44) 21 (22) 70,34 (40,63) 1,67 (27,25)					1,67 (27,25)
Number of necessary labour per day 70 (81)					
Total pr	roduction of man	ufacture [pi	ieces]	14019	(6230)

Tab 5: Report on Results of experiment No.1

Tab 6: Report on Results of experiment No.2

Report on individual workplaces					
Workplace No.	Description of workplace	Number of machines	Number of shifts	Busy Time [%]	Blocked Time [%]
1	Drilling	2 (3)	1 (2)	96,99	0,00
2	Countersinking	1	1 (2)	86,95	0,00
3	Turning-Lathe – Fischer	3	2	67,55	0,00
4	Turning-Lathe - SV 18	7	3 (2)	93,07	0,00
5	Turning-Lathe - Liberty	6	2	84,60	0,00
6	Honing	2	3 (2)	76,17	0,00
7	Forging	2	3	93,40	0,00
8	Grinding	6	2	84,99	0,00
9	Turning-Lathe – chambers	3	3 (2)	94,49	0,00
10	Polishing - chambers	2	2	64,66	0,00
11	Manual treatment	1 (9)	1	15,73	0,00
TOTAI		35 (44)	23 (22)	78,05 (40,63)	0,00 (27,25)
Number of necessary labour per day			80	(81)	
Total production of manufacture [pieces]20140 (6230)				(6230)	

Experiment No.2

Experiment No.2 tries to remedy the critical points of the previous experiment. Results in Table 5 show that it is necessary to increase manufacturing capacity of Turning-Lathes–SV18 and Turning-Lathes – chambers. Solution to this problem is setting the working shifts of these workplaces in three-shift operation. Results of this simulation experiment are shown in Table 6.

More than treble Total production increase at the practically identical labour (80 labourers) is reached in this experiment. Blockage of the machine almost never occurs. Imperceptible blocking of the Turning-Lathes-Liberty comes about after one month simulation.

Experiment No.3

Experiment No.3 solves lower workload of Turning-Lathes – Liberty, workplace of grinding and workplace of Polishing-chambers. The number of Turning-Lathes-Liberty and grinding machines is decreased. The workplace of polishing-chambers is set in three-shift operation but the number of machines is reduced.

Results of this simulation experiment are shown in Table 7. Five labour positions are saved compared to the previous experiment. Value of Total production is practically unchanged. Imperceptible blocking of the Turning-Lathe-Liberty comes about after two month simulation.

Tab 7: Report of	on Results o	of experiment	No.3
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	Report on individual workplaces					
Workplace No.	Description of workplace	Number of machines	Number of shifts	Busy Time [%]	Blocked Time [%]	
1	Drilling	2 (3)	1 (2)	96,99	0,00	
2	Countersinking	1	1 (2)	86,95	0,00	
3	Turning-Lathe – Fischer	3	2	66,83	0,00	
4	Turning-Lathe - SV 18	7	3 (2)	90,89	0,00	
5	Turning-Lathe - Liberty	5 (6)	2	95,20	0,00	
6	Honing	2	3 (2)	75,93	0,00	
7	Forging	2	3	91,80	0,00	
8	Grinding	5 (6)	2	95,54	0,00	
9	Turning-Lathe – chambers	3	3 (2)	94,51	0,00	
10	Polishing - chambers	1 (2)	3 (2)	87,61	0,00	
11	Manual treatment	1 (9)	1	15,74	0,00	
TOTAL 32 (44) 24 (22) 81,64 (40,63) 0,00 (27,25)					0,00 (27,25)	
Number of necessary labour per day 75 (81)					(81)	
Total pi	roduction of man	ufacture [pi	eces]	20146	(6230)	

Experiment No.4

Experiment No.4 corresponds practically to experiment No.3. This experiment corrects the lower workload of Turning-Lathes - Fischer. The number of machines in this workplace is reduced. Results of this simulation experiment are shown in Table 8.

Total production increase (cca 120 pieces) and labour cut (1 labourer) are achieved compared to experiment No.3. However Turning-Lathes-SV18 are blocked soon (after 3 weeks). It is resulted from maximum busy time of Turning-Lathes-Fischer.

1 au o. Report on Results of experiment no.	Tab	8:	Report	on	Results	of	experiment No.4
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	Report on i	ndividua	l workpl	aces	
Workplace No.	Description of workplace	Number of machines	Number of shifts	Busy Time [%]	Blocked Time [%]
1	Drilling	2 (3)	1 (2)	96,99	0,00
2	Countersinking	1	1 (2)	86,95	0,00
3	Turning-Lathe – Fischer	2 (3)	2	97,00	0,00
4	Turning-Lathe - SV 18	7	3 (2)	89,38	0,00
5	Turning-Lathe - Liberty	5 (6)	2	95,87	0,00
6	Honing	2	3 (2)	79,18	0,00
7	Forging	2	3	95,87	0,00
8	Grinding	5 (6)	2	95,61	0,00
9	Turning-Lathe – chambers	3	3 (2)	95,05	0,00
10	Polishing - chambers	2	2	65,05	0,00
11	Manual treatment	1 (9)	1	15,83	0,00
TOTAL 32 (44) 23 (22) 82,98 (40,63) 0,00 (27,25)					0,00 (27,25)
Number	Number of necessary labour per day 74 (81)				
Total p	roduction of man	ufacture [pi	ieces]	20263	(6230)

Experiments Evaluation

On the basis of the results of executed experiments (see Table 5, 6, 7, 8); we can say that Experiment No.4 is the best. Total production of manufacture is the highest and labour cuts (7 labourers) are achieved. However this experiment has a weak point which comes out after longer simulation time. Turning-Lathes-SV18 are blocked after 3 weeks. It is resulted from maximum busy time of Turning-Lathes-Fischer. From this point of view it is better Experiment No.3. Blockage of the machines almost never occurs. Imperceptible blocking of the Turning-Lathe-Liberty comes about not until after two month simulation time. Six labour positions are saved compared to the current manufacturing line. Value of Total production is practically comparable to Experiment No.4.

CONCLUSION

This paper presents possibilities of utilization of dynamic simulation when searching for reserves of the manufacturing systems. On a concrete example, utilization of the simulation Witness environment is demonstrated in the suggestions for increase of production efficiency in the company manufacturing the short barrels of the gun. On the basis of many simulation experiments, it was corrected bottlenecks of the current manufacturing line. Solution consists in elimination of some machines in the selected workplaces. For other workplaces, it was suggested to reduce eventually to increase the number of shifts of the operation. All the suggestions result not only in increase of manufacture production (in our case not less than 1000 pieces a day) but also in savings of labour and energies.

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A FLEXIBLE APPROACH FOR THE DESIGN OF A MULTIMODAL TERMINAL SIMULATION MODEL

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KEYWORDS

Multimodal transport, terminal simulation, flexible design.

ABSTRACT

We present a decision support tool for the analysis and redesign of railroad intermodal terminals. It is a simulation-based platform which provides indicators of service level, resource use and productivity linked to the terminal operations and infrastructures. The platform is composed of two basic elements: a simulation model implemented in a commercial simulator, Witness®, and a configuration interface implemented in MS Excel®. The combination of these components has facilitated building a very flexible and easy-to-use platform so that a user without any knowledge of the simulation software will be able to implement a simulation model of the terminal, by only filling in the required data through an MS Excel file. As the design of the platform has focused on flexibility, a wide range of terminals can be implemented, in terms of infrastructures, handling material, lay out and train and demand patterns. We also present a case study to demonstrate the use of the platform.

1. INTRODUCTION

Despite the well-known benefits that could derive from the use of intermodal transport (energy efficiency, reduced road congestion and environmental damage...), the choice of a transport mode relaies on the existence of a guarantee of the effectiveness and efficiency of the transport service. Thus, it is critical to analyse the transport chain from a global perspective in order to identify the bottlenecks and other barriers that may be preventing the development of combined transport.

We believe that simulation may play an important role in the development of the necessary quantitative tools, to analyse transport networks. However many times, the gap between researchers and managers has been a burden for the use of simulation in real life problems. Therefore, in this research project we have focused on the design and development of a flexible and easy-touse simulation platform.

In an intermodal chain many factors critically affect performance, and one of them is the operations that take place in the transhipment terminals. Therefore, the study

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) and optimization of terminal operations has been the object of many research works, especially in the last two decades.

Many simulation models have been proposed to study terminal operations from a holistic perspective. For example, Shabayek and Yeung (2002) propose a deterministic model implemented with Witness, which provides for indicators of resource use in Hong Kong's container terminal. Similarly, Cortés et al. (2007) show a simulation model implemented with the commercial software Arena, which represents the operation of the Port of Seville in detail, including the processes regarding truck management (entering/exiting the terminal and loading and unloading operations); ship allocation, unloading/loading arrival and dock operations, etc. The simulation delivers results regarding infrastructure and resource use, truck flow and vessel throughput time.

These two research works are good examples of the benefits of using simulation to study the performance of a specific terminal. However if the study is to be extended to an entire network, a more flexible model design of the model, such us the one we present, could be more appropriate, as the total development cost of the model would be significantly reduced. Moreover, the study of a variety of scenarios often requires a substantial modification of the model code, if flexibility has not been introduced as a design requirement of the model. With the proposed approach, many of the changes that could be introduced to implement the alternative scenarios would be trivial.

To stablish the research objectives of this work we have chosen to focus on the simulation of railroad terminals in a rail network, thereby developing a simulation platform based on the combination of Witness, as the simulation software, and MS Excel to develop the user interface. The details of the research work are structured as follows: In section two, we describe the system studied in terms of infrastructures, resources and operations. This conceptualization leads to the specifications of the model and the programming strategy adopted, which are explained in section 3. In section 4 we present a case study that illustrates the use of the simulation platform. Finally, in section 5 we summarize the conclusions of this research.

2. TERMINAL CONCEPTUALIZATION

There are a wide variety of terminals with various characteristics: localization, modes of transport involved, volume of transhipments. These characteristics introduce differences among them which have to be carefully analysed to assess their potential impact on the model flexibility.

The most significant criterion for classifing terminals is probably the number of modes involved in transhipment operations. Regarding this criterion, we may divide the rail network terminals into two categories: marine and interior terminals. In the first type, there are potentially three transportation modes involved (sea, rail and road), whereas in the second entails, only rail and road modes.

In this research, we have chosen to focus on interior terminals for several reasons. First, they are less complex than marine terminals, and thus they constitute a better starting point for the development of the simulation platform. Secondly, they have received less attention in the related literature than the maritime ones. Finally, after a careful analysis of their characteristics, they seem to provide a reasonable balance between a variety of characteristics (which justifies a flexible approach), and common aspects (which facilitates a successful implementation).

The experience gained in this first work will be used to extend the model approach to the implementation of maritime terminals.

The interior railroad terminals modelled perform the following main processes:

- Truck arrival and departure.
- Truck loading and unloading.
- Container reception and storage.
- Train arrival and departure.
- Train loading and unloading.

To accomplish these processes, a variety of infrastructures and resources are used. We present below a brief description of them. Figure 1 shows a scheme of these resources and their connections:

- Entry and exit gates used by the trucks.
- Truck loading and unloading positions.
- Truck parking area. This is a FIFO queue used when all the loading/unloading positions are in use.
- Stacking areas. We have considered two types:

- Long-term stacking yards. Most of the terminal storage capacity is concentrated in these yards. In the cases studied, these yards are separated from the train loading/unloading area and containers have to be handled by mobile cranes.
- Short term stacking lines. Containers are stored in lines on both sides of the loading/unloading tracks. These lines may usually be reached by the loading/unloading gantry cranes.

We have included both types of stacking areas in the model. The containers are generally stored in the long-term stacking yards. Short-term stacking lines are reserved for those that are to be delivered in less than 24 hours.



Figure 1: Scheme of Terminal Infrastructure and Operations

- Terminal Enter/Exit tracks. We have assumed that the terminal has one entry track and one exit track, which are used by the trains to enter and exit the terminal.
- Reception/expedition and loading/unloading tracks. We have considered that all these tracks can assume any of the functions depending on the needs at any given time.
- Cranes, used for truck loading and unloading, to manage the stacking yards and for train loading and unloading. Usually there are two types of cranes in interior terminals with a certain container volume: gantry cranes and mobile cranes. In the Spanish case (which has been the reference for many design aspects), gantry cranes are usually reserved for train loading and unloading. In fact, they are normally attached to the loading/unloading tracks and can only move along them, thereby making transhipments between trains and the short-term stacking yards. Mobile cranes may be used for all

the loading/unloading operations that take place at the terminal. Therefore, we evaluated two alternatives:

- Using gantry cranes for train loading and unloading and mobile cranes for these two operations and also for truck loading and unloading and operations in the long-term stacking yards.
- Specialized functions: the gantry cranes would have the same use as in the former alternative, and mobile cranes would only be used for truck loading and unloading and operations in the long-term stacking yards.

We adopted the second alternative because we estimated that the use of mobile cranes for the same function performed by gantry cranes would be a rather unusual situation, which could just be omitted in the simulation.

- Diesel engines, which are in charge of the train movement inside the terminal.
- The human personnel who operate the terminal have not been considered explicitly, as most of them are crane operators. Moreover, cranes are scheduled following operator shifts and therefore, operator activity may be monitored through the performance measures linked to crane use.

3. DESIGN AND IMPLEMENTATION OF THE SIMULATION PLATFORM

The first decision regarding platform design is the choice of simulation software. In this case, this decision did not require much analysis because the research team had substantial experience with the use of Witness to develop combined transport models (see García and Gutiérrez, 2003; Marín et al., 2004). In those situations the software had performed very well. Additionally, the fact of having previous knowledge of the software was another point in its favour.

The decision about the user interface was more complicated and required the comparison of various approaches. Two of them were thoroughly explored:

- The use of Witness utilities, mainly modules and dialogue boxes.
- A MS Excel file appropriately combined with the Witness model.

After comparing them, we chose the second alternative, mainly because its implementation seemed faster and more robust and because it permits defining a terminal model for any user regardless of simulation language.

The starting point for the platform design was the conceptualization described in the previous section.

Each of these elements was analysed in detail in order to establish the model specifications regarding it. The aim was to obtain the right balance between flexibility and specifity. For example, the number of mobile cranes is one of the characteristics that changes from one terminal to another. Therefore, the platform should allow the user to establish the number of mobile cranes at a terminal. At the same time, the more flexible the model design is, the more complex the model programming becomes. In this case, the right equilibrium was reached in allowing the user to establish the number of gantry cranes for any quantity between 0 and 8.

Another feature of the simulation platform is related to the use of modules. The terminal operations may be divided into functional areas, according to the terminal activities mentioned in the previous section. We have identified five areas, each of which led to a module:

- Truck loading and unloading module.
- Train loading and unloading module.
- Container reception and storage module.
- Long term stacking yard module.
- Mobile cranes module.

All these modules are programmed to leave most of the defining elements expressed as parameters, the values of which shall be entered by the user through the MS Excel file.

The MS Excel file reproduces the same structure as the Witness model, using a separate sheet for each module.

In the next two subsections, we explain in greater detail the two main building blocks of the platform.

3.1. Witness Simulation Model

We present below a brief explanation of the main activities simulated by the model.

- Truck unloading. The trucks arrive at the terminal according to a stochastic arrival pattern, defined by the user. The truck enters the terminal and if possible, occupies an unloading position. In the case that all positions are taken, it waits in the terminal parking area until a position is available. The unloading process only begins when the truck is in the unloading position and a mobile crane is available to perform the task. When the unloading task is finished the truck leaves the terminal and the mobile crane transports the container to the appropriate stacking yard.
- Truck loading. This process is rather symmetrical to the unloading process described bellow. The main difference is that the truck arrival generates a

search order for the appropriate container that is executed as soon as a mobile crane is available.

Figure 2 shows the truck loading and unloading module.



Figure 2: Simulation Model – Truck Loading and Unloading Module

- Train unloading. Trains arrive at the terminal according to a fixed schedule. The train enters using a single entry track. Afterwards, the electric engine is substituted by the diesel engine, which carries the train to an available loading/unloading track. The unloading process is performed by a gantry crane and the containers are provisionally stored in the short-term stacking lines. Next, mobile cranes transport the container to the long-term stacking yard or to the truck loading area.
- Train loading. The trains also leave the terminal according to a fixed schedule. When the remaining time for train departure reaches the limit specified a loading order for the train is generated. The containers that are to be loaded are transported from the long-term stacking yard to the short-term stacking lines. Subsequently, the gantry cranes transfer the containers from the stacking lines to the train. When the loading process is finished, the electric engine is fixed and the train waits until departure time.

The results provided by the simulation may be grouped into three sets: service level, productivity and resource use. Service level results arising from the model are, for example: the number of trains per week which fail to be loaded, average and maximum waiting time for trucks, average and maximum container time at the terminal. Terminal productivity is measured by the number of loaded and unloaded trucks per day and the average train length (in number of containers). Finally, the model quantifies the use of the terminal resources: gantry and mobile cranes, engines, stacking areas, loading/unloading tracks and parking areas.

3.2. User Interface. MS Excel File

The user interface is implemented through a MS Excel file. The file is structured by sheets, each of which correspond to a Witness module. All the data necessary to define the infrastructure, demand, train schedule is introduced by the user through this MS Excel file and the user does not need to do any programming work in Witness. Once all the required data is filled in, the user can just open the Witness file and run the simulation.

The file is structured as follows:

- General data: Terminal layout, load reception hours, maximum number of destinations...
- Truck loading/unloading area: Number of gates, entry processing time, parking capacity, number of loading/unloading positions and truck arrival distributions.
- Train loading/unloading area: trains timetable, number of tracks, advance before the scheduled departure for the train loading and minimum and maximum length of trains.
- Mobile cranes: number of cranes, work shifts, crane speed, container loading and unloading time.
- Gantry cranes: number of gantry cranes, container loading and unloading time.
- Diesel engines: number of engines, working shifts, speed and time required to change between electric engine and diesel engine.
- Stacking areas: stacking area dimensions and maximum stacking height.

The aforementioned time data may be defined as determininate parameters or as random distributions.

As an example, in the case of the input of the number of mobile cranes, Figure 3 shows the manner in which the MS Excel interface and the Witness model are linked. In the Figure's upper left corner the MS Excel is shown. The MS Excel sheet provides a brief explanation about the parameters that must be entered by the user. The table shows the three default values, which may be changed by the user, for the three required parameters: number of mobile cranes that work one, two or three shifts. The right lower corner of Figure 4 shows the code that creates the specified number of mobile cranes in the Witness model.



Figure 3: Data Input for the Number of Gantry Cranes

The user interface has been furnished with many utilities which prevent it from making mistakes in the data input process: explanations about the data required, error messages that display when the input introduced is incorrect, links between sheets which help follow the right order and protecting instruments so that the sheet structure cannot be modified.

4. CASE STUDY

In this section, we present an application of the simulation platform used to study the capacity of a terminal. The case study is based on an existing container terminal in Spain.

4.1. Simulated Scenario

The terminal studied has the following resources and infrastructures:

- Two entry gates and two exit gates for trucks. The time spent by trucks at these gates follows a random empirical distribution, varying between 4 and 6 minutes.
- The parking area has a maximum capacity of 4 trucks. The parking area is used in the case that all the loading/unloading positions are occupied.
- The long term stacking area has a maximum capacity of 440 ITUs, and the short-term stacking lines have a maximum capacity of 180 ITUs.
- One entry track and one exit track. Four loading/unloading tracks and one diesel engine.
- Two gantry canes and two mobile cranes the processing times of which have been represented as random empiric distributions.

The terminal exchanges containers with four nodes of the rail container network and distributes and receives road traffic within its own region. The destinations are coded by indexes D=i, i=1...5. The outgoing road

traffic is named D=1 and the subsequent indexes, 2 to 5, correspond to the four destination rail terminals.

The incoming (I) and outgoing (O) trains follow the schedule shown in Table 1. For the outgoing trains, the table specifies the destination index.

	Mon	Tue	Wed	Thur	Fri	Sat	Sun
1:40		Ι	Ι	Ι	Ι	Ι	Ι
6:35		O 2	O 2	O 2	O 2	O 2	O 2
9:10	Ι	Ι	Ι	Ι	Ι		
10:00	O 3		O 3		O 3		
13:12	Ι		Ι		Ι		
21:20	O 4	O 4	O 4	O 4	O 4		
21:40						Ι	

Table1: Train Timetable

The loading order is opened 120 minutes prior to the train departure and it is closed 20 minutes prior to it. A loading order will only be accepted if there is a minimum of six train platforms to be loaded.

Truck traffic is approximately 80 trucks a day, including both delivery and collection flows. The arrivals of the trucks distribute randomly with a daily seasonality.

4.2. Results Analysis

We have simulated the previously-described terminal operation. The duration of the simulation was one week. As some of the inputs are stochastic variables, we carried out five replications.

The results demonstrate a low or very low use of the terminal equipment. As shown in Table 2, the average percentage of total time that the two mobile cranes are used (MC) is nearly to 40%. The percentage of time that the two gantry cranes are used is even lower: approximatelly 13%. Finally, the use of the diesel machine that moves the trains inside the terminal is just occasional and represents less than 2% of total time.

Table 2: Use Percentage of Terminal Equipment

	MC	GC	DM
Rep1	40.38	13.16	1.33
Rep2	39.86	12.72	1.3
Rep3	39.82	12.64	1.41
Rep4	40.05	13.14	1.47
Rep5	39.23	12.29	1.36
Average	39.87	12.79	1.37
S.D.	0.42	0.37	0.07

Similar results are obtained regarding to the use of infrastructures. Table 3 shows the average and standard deviation obtained for the five replications for the use of entry and exit gates of the terminal (both occupied around 14% of total time), the trucks loading/unloading

positions, which are used only 5.3% of total time and the tracks, which are used about 12% of total time.

Table 3: Infrastructures Percentage of Total Time Used

	Average	S.D.
Entry Gates	14.05	0.22
Exit Gates	13.97	0.23
Load/Unload	5.345	0.06
Tracks	11.85	2.05

This resource availability leads to good results in terms of service quality. For example:

The waiting times in the truck loading/unloading module are small. As we explained before, there is a parking area where trucks may wait to be processed if all the loading/unloading positions are occupied. As shown in Table 4, the average value for the waiting time in this parking area is 1.06 Once is an available minutes. there loading/unloading position, the truck waits an average time of 2.57 minutes for the mobile crane to arrive if it is waiting to be loaded, and an average of 1.66 minutes, if it is waiting to be unloaded. The fact that waiting time for the loading process is higher than the waiting time for the unloading is consistent with the model hypothesis, as the former involves the additional operation of finding the container to be loaded in the stacking area.

Table 4: Waiting Times in the Truck loading/Unloading Module (Minutes)

	Average	S.D.
Parking	1.06	0.75
Loading	2.57	0.11
Unloading	1.66	0.26

- The performance indicators associated with train loading/unloading processes also have satisfactory values: As we show in Table 5, the average time employed in train loading is 175.6 minutes and the mean time for train unloading is 35.64 minutes.
- The average container delay at the terminal is high: approximately 45 hours. This value is related to train frequency and the destination of containers.
- Finally, the average number of containers on a train is relatively high: 24 containers.

Table 5: Results of the Train Loading/Unloading Module

	Average	S.D.
Loading (min)	175.56	3.26
Unloading (min)	35.64	0.65
Number of Cont.	24.11	1.37

Even if the general picture of the terminal performance shows a clear resource availability in average values, the simulation has revealed that the system also has some peaks that occasionally cause resource overload:

- We have observed some punctual demand peaks, which cause overloading at some terminal points. For example, sometimes the influx of trucks is too high to be managed at the entry gates and some trucks are rejected. As shown in Table 6, the absence of a queue outside the terminal, causes at these peak moments the rejection of 6 trucks which intend to unload containers and 1.6 trucks that are coming to pick up containers.
- The mobile cranes have also experienced overload, which causes transitory blocking in the container transhipments between the long-term stacking yard and the short-term stacking lines. In this model, mobile crane overloading leads to the rejection of some loading orders, namely, an average of 3.2 orders, considering the five replications (see Table 6).

Table 6: Number of Trucks and Trains Rejected

	Average	S.D.
Trucks for loading	1.60	0.55
Trucks for unloading	6.00	0.00
Trains for loading	3.20	1.10
Trains for unloading	0.00	0.00

5. CONCLUSIONS

We have presented a simulation platform that is designed to leave most of the infrastructure, demand and resources characteristics in a parametric form, so that the user may implement a wide range of different terminal configurations by only entering the required data into a very easy-to-use interface. This flexible approach is especially useful in generating various scenarios in the terminal redesign process easily and quickly. It can also be very interesting when the objective is to create a network model with many different terminals.

To illustrate the use of the platform, we have implemented a case study where a terminal is represented. We have measured the terminal performance in terms of average values, but we have also studied the exceptional moments when resources become overloaded.

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A DISCRETE EVENT SIMULATION MODEL FOR THE ANALYSIS OF CRITICAL FACTORS IN THE EXPANSION PLAN OF A MARINE CONTAINER TERMINAL¹

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KEYWORDS

Discrete Event Simulation; Marine Container Terminal; Performance analysis.

ABSTRACT

In this paper we present a discrete event simulation model to approach the decision problems arising from an expansion plan of a marine container terminal. In particular the preliminary study herein presented starts from a collaboration with the Southern European Container Hub (SECH) sited in the Port of Genoa, Italy. The planned expansion will take place from 2010, the terminal area will enlarge, thus being capable of doubling the present TEU handling capacity. Due to the foreseen increase in the traffic volume, there is the need of defining new management policies, mainly related to the organization of the yard and quay sides of the terminal. The proposed simulation model, that has been implemented by the Witness software environment, can be used to analyse different scenarios, pertaining to possible changes of the import/export flows, handling techniques, different equipments and investment options as well as different operative rules for the berthing and storage area.

INTRODUCTION AND PROBLEM DEFINITION

The steady increasing number of container shipments is causing higher demands at the seaport container terminals, and, consequently, the competition among seaports is increasing too, especially among geographically close ones. The competitiveness of a marine container terminal is based on different factors, such as ship turnaround time, number of TEUs moved per unit of time, combined with low rates for loading and discharging and fast turnover of containers.

In general terms, an import/export container terminal can be described as an open system with two external

interfaces: the quayside, or marine side interface, with loading and unloading of ships, and the land side interface where containers are moved from/to trucks and trains. A container vessel, after its arrival at the terminal, is assigned to a berth equipped with quay cranes for loading/unloading operations. The import flow starts with unloading operations from the ship; the unloaded containers are transferred by internal transportation equipment, i.e. vehicles, multi-trailers, fork lifts (FL), straddle carriers (SC) or Reach stackers (RS), to the storage area (yard) for their later departure via trucks or trains. In the yard they are stored in stacks using rail mounted gantry cranes (RMG) or rubbed-tired gantry cranes (RTG). Different storage strategies can be used by the terminal yard management i.e. the premarshalling strategy and the sort and store strategy (see e.g. Ambrosino and Sciomachen (2003)). The export flow concerns containers that reach the terminal via trains or trucks, are stored in the yard by using dedicated equipment (see e.g. Vis and Harika (2004) for an overview of vehicle types at a container terminal) and finally are loaded on board for their departure by ship.

In general, a marine terminal must be managed in such a way to optimise the collective flows of containers that arrive and leave it via trucks, trains and vessels. An expansion plan can affect the efficiency and the "optimal" management of the whole terminal, thus requiring to analyse the emerging critical factors in the terminal system.

In the following we will deal with the issues arising from an expansion plan of a import/export container terminal sited in the Port of Genoa, Italy that is the Southern European Container Hub, SECH. Following the planned expansion, that will take place from 2010, the terminal area will enlarge from 207.000 to 480.000 sqm, thus making the terminal able of doubling the present TEUs handling capacity.

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In Figure 1 is depicted the planned change of the terminal layout. Interested readers can refer to the web site <u>http://www.sech.it</u> for getting more information about the terminal SECH and its expansion plan.

Terminal design problems, related to the multi-modal interfaces and the equipment type selection, have been approached by facility planners in the first stage of the terminal expansion (see the input data analysis section). The organization of the yard and the quay operations should be revised to be able to meet the new foreseen increased traffic of containers. Terminal managers need to test and compare different new management policies. Their goal is both improving the terminal productivity by a better synchronization among the handling facilities and achieving cost savings related to a better usage of handling and human resources.

For this purpose, using the Witness software environment, we have developed a discrete event simulation model. This model can be used for different "what-if" analysis pertaining to possible changes of the import/export flows, handling techniques and equipment, as well as different operative rules for the quay side and yard area.



Figure 1. Layout of the SECH: old and new area

A container terminal includes a multitude of interacting factors (e.g. ship, truck and train arrival patterns, various kinds of cargo-handling equipment and human resources) and the randomness and complexity of the problem under consideration make the analysis of a marine terminal an interesting ground for applying simulation models.

We evaluate the terminal performance by analysing some indices of interest, such as the so-called net terminal performance index, the average yard and quay utilization rate and rotation index (Petering and Murty 2009). Moreover, we focus our attention to a "gang utilisation rate", that we use for defining the shifts of the personnel closely related to the container handling operations from the sea side to the land one, and viceversa.

The paper is organized as follows. A literature review about the use of simulation for optimising the logistic

operations at container terminals is reported in next section. Afterwards we focus on the modelling approach and the development of the simulation model, with particular attention to the data analysis and estimation. Finally, conclusions and further work are discussed.

LITERATURE REVIEW

Due to the continuous growth of the container flow over the world, container terminal operations are becoming more and more important in the search for terminal competitiveness. Therefore, there is an ever-increasing number of publications on container terminals showing the need for an optimal management of their logistic activities.

Vis and De Koster (2003) and Steenken et al. (2004) give a classification of the decision problems at marine container terminal in accordance with the following logistic processes: *i*) arrival of the ship, *ii*) discharging and loading of the ship, *iii*) transport of containers from ship to stack and vice versa, *iv*) stacking of containers, and *v*) inter-terminal transport and other modes of transportation.

Moreover, Gunther and Kim (2006) propose a classification of these problems in accordance with the planning level they are related to. In particular, the strategic level refers to long-term decisions pertaining layout, connections, equipment, berthing and yard capacity, the tactical level regarding mid-term decisions pertaining berth and yard planning and policies, while the operational level pertains to short-term decisions related to the quay side and land side operations.

By using an integrated classification, a quite complete list of decision problems to be solved at marine container terminals (MCT) is summarized in Figure 2.



Figure 2. Problems and decisions at MCT: An integrated classification

Most researchers deal with these problems decomposing the complex system into sub-systems and approaching single decision problems separately, i.e. berth allocation problem (Imai et al. 2002, Cordeau et al. 2005), quay crane assignment problem (Zhang et al. 2002), ground crew planning problem (Legato and Monaco 2004), optimal sizing of storage space and handling facilities (Kim and Kim 2002), stacking strategies (Kang et al. 2006), etc. Other authors propose decision support system, simulation model and queuing models, to study the terminal as a complex system consisting of several integrated and correlated sub-systems (Gambardella et al. 1998; Bingham et al. 2003; Legato et al. 2008; Canonaco et al. 2008). Recently, simulation approaches have been quite often used for testing design and structural parameters affecting the performance and productivity of real marine terminals. Parola and Sciomachen (2005) study the whole logistic inter-modal network among ports and consider marine terminals as single nodes in the given simulation model aimed at evaluating possible growths of the rail connections, while Parola and Sciomachen (2008) approach the modal split evaluation at terminal VTE in Genova (Italy). Nam et al. (2002) examine the optimal number of berths and quay cranes for a terminal in Busan (Korea), while Legato and Mazza (2001) develop a simulation model for the arrival-departure process of vessel at the container terminal of Gioia Tauro (Italy) that is used for optimisation scenario analysis of the berth planning problem. Shabayek and Yeung (2002) describe a simulation model to analyse the Kwai Chung container terminals in Hong Kong, that has been proved to predict the actual container terminal operations with a high order of accuracy. Kia et al. (2002) describe the role of simulation for evaluating the performance of a terminal's equipment and capacity in Melbourne by using interesting performance criteria and model parameters.

In the following we focus our analysis on strategic and tactical decision problems pertaining to a terminal expansion. In particular, we deal with the problem of organizing the berthing and storage area.

We present preliminary results of a collaboration project aimed at developing a discrete event simulation model to support the terminal management during a planned terminal expansion.

MODEL DEVELOPMENT

Data collection and analysis

The terminal SECH is a medium sized import export container terminal based upon the "Indirect Transfer System" (ITS) in which a fleet of shuttle vehicles transports the containers from a vessel to the stack area and vice versa, whilst dedicated cranes (i.e. rail mounted gantry cranes (RMG) or rubbed-tired gantry cranes (RTG)) stack or pick up containers in the yard slots. Export containers arriving by road or railway at the terminal are handled within the truck and train operation areas, picked up by the internal transportation equipment and distributed to the respective stacks in the yard by using dedicated equipment. The terminal is situated within the Port of Genoa. Its total area is 206.000 sqm, the yard area is 13.000 sqm and the quay length is 526 m, corresponding to an handling capacity of 450.000 TEUs (Twenty Equivalent Units) per year. Note that the strategic decisions (layout, connections, equipments, berthing and yard capacity) have been modelled following the facility planners' decisions pertaining to the enlargement plan that will take place from 2010.

Table 1 and Table 2 gives the current (Year 2008) and planned (Year 2010) terminal capacity (yard, quay, rail and gate connections) and equipments, their number, and movements / hour, respectively.

Table 1. SECH facilities (2008-2010)

	Year 2008	Year 2010
Total surface	206.000 sqm	480.000 sqm
Yard capacity	13.000 teu	24.500 teu
Quay length	526 m	526 m + 760 m
Rail	3 tracks	9 tracks
Gate	5 reversible lines	10 reversible lines

Table2. SECH handling equipments (2008-2010)

	Year 2008		Year	2010
Equipment	Q.ty	Speed (mov/h)	Q.ty	Speed (mov/h)
Portainer	5	18/19	11	18/19
RMG	6	18	6	18
RMG*	-	-	20	20
RTG	8	16	8	16
Reach stacker	16	14	16	14
Fork lift	8	14	8	14
Internal truck	27	60 Km/h	37	60 Km/h

When studying a marine terminal system, one of the major problems is the difficulty in getting the large amount of data necessary to build a representative model and record the data in a format usable for the statistical parameters estimation. Moreover, in our study an additional problem pertains to the unavailability of the data regarding a "future" situation. For our analysis we decided to start with the real data collected during the time period January 2007-December 2007, and to adjust them following the terminal managers' forecasting.

In particular, the main data are related to: a) the ship inter-arrival time and turnaround time; b) the quay crane service time; c) the truck and train inter-arrival times and d) internal transport and yard stacking equipment service times.

Note that the ship turnaround time includes the ship arrival, the waiting time before using the terminal facilities and the berthing time (service time). The number of available berths is an obvious factor in determining possible queues. The available statistics related to the arrival-departure process of the ships served by SECH gives for each month the number of ship entered, the average time of berthing and unberthing, the total number of full and empty containers discharged and loaded and the number of restowages which occurred, respectively, during the loading and unloading operations. These reports have been used for obtaining the distributions of the ship inter-arrival time belonging to four shipping services denoted AME, EMA, MIX and NEW. For each service we suppose a negative exponential distribution of the ship inter-arrival times, as it is commonly used (Kia et al., 2002). Finally, using the data provided by the SECH about the handling moves for each vessel, i.e. min, max and mode, we defined a triangular distribution for generating samples of discharging, i.e. import container moves, and loading activities, and a T-normal distribution with a lower and an upper bound, related to the minimum and maximum number of cranes assigned to each ship. The export containers arrive both via trains and trucks. Since the rail modality has a great importance in the model, in our analysis we decided to focus our attention on both block trains, which represent a large part of the volumes transported via rail, and normal singular trains.



Figure 3. Relative frequency of train inter-arrival times: official timeline versus real data

For studying the arrival process of containers by trains we used the official timeline of the Railways national company and computed the corresponding inter-arrival times split into time slots of 30 minutes each. Note that the official timeline differs from the real trains arrival (real data) profiles observed in the study period (see Figure 3), but in both cases, by using a Chi square test at 90% confidence level, polynomial distributions appear acceptable for modelling the trains' arrival process.



Figure 4. Average distribution of daily trucks' arrivals

Lastly, the time that each truck spends at gate is defined by a triangular distribution that is extrapolated by information of the stevedores, as well as the data concerning the truck arrivals during the day split into 48 time period of 30 minutes each (Figure 4).

Modelling approach and implementation

The discrete event simulation model herein proposed is made up of three modules: the ship flow module, the import container flow module and the export container flow module. These modules manage the action sequence of model objects (ship, import and export containers) through a given series of logistic processes (Figure 5).



Figure 5. Model hierarchy structure



Figure 6. Flow chart of the import flow module

Each module is represented by a flow chart, where activities and events that compose the module are nodes of the graph and edges fixing the logical sequence among nodes. In Figure 6 is reported the hierarchical flow chart referred to the import flow module. Note that for each node, a simulation quasi-language provides the simple activities and events specification as input or output rules.

Those rules can be viewed as the declaration of the solution of the different decision problems to be solved at a marine terminal (Figure 2). As an example, Figure 7 shows the representation of the storage policy followed at SECH to stack import containers that is a pre-marshalling strategy, i.e. containers are stored in different areas in accordance to their weight (W), type, shipping company and size.



Figure 7. Representation of the storage policy strategy

The model has been implemented using the simulation software package Witness 2008 (Witness, 2008), that is a flexible visual-interactive environment that allows defining an animation along with the model construction. Model objects, denoted parts, pass through the system according to the module flow charts, from/to queue (i.e. buffers), and are processed by machines that perform some specified activities. Inter-arrival times and service times have been modelled by following the information obtained from the data analysis presented in the previous section. The Witness model implementation is shown in Figure 8, where the basic elements are depicted as they appear on the computer screen. Note that the model implementation results in 7 model objects (4 ship services, trains, import and export containers), 208 buffers, 175 machines, 15 empirical distributions, 75 among variables, attributes and functions for a total number of 489 elements.

Model validity and credibility

Once a simulation model has been constructed and implemented, it need to be validated to ensure that the simulation outputs adequately represents the real measures under investigation. In our case study the model to be validated represents a system that doesn't currently exist (the terminal SECH in 2010), thus we can't get the real output data to apply statistical tests techniques. Consequently, the effective and strong method of the results validation has to be replaced by the face validation (Law, 2007). In particular, the terminal managers review the simulation model for reasonableness and test if the simulation results are consistent with the perceived system behaviour of the SECH container terminal resulting from the expansion plan.



Figure 8. The simulation model Witness representation

Moreover, to improve the model credibility, we decided to validate the model related to the current layout (the "old area" in Figure 1) by using quantitative techniques. In particular, we used a classical statistical test, such as the t-Test, for comparing three monthly output measures, i.e. average estimates of ship arrivals, containers' arrivals by train and trucks, with the real measures related to the period January-December 2007. We decided to test the null hypothesis H_0 under a probability of rejecting the model fixed to the α =0.05 level, obtaining for all months values inferior to the critical value.

Output analysis: performance indexes and running configuration

For the output analysis, we focus our attention on two series of performance indexes: i) the service-oriented indexes that measure the service levels provided to clients, and ii) the productivity-oriented indexes that measure the container traffic volume internal performance.

In the first group the most important indices are: 1) the average ship berthing time; 2) the so-called net terminal performance index, expressed in terms of the ratio between the total number of containers moved from each ship and the berthing time, and 3) the average container dwell time, i.e. the average time spent in the system, both for import and export containers. When referring to the productivity-oriented indexes we can mention: 1) the import and export container throughput, i.e. number of containers that leave the system during the simulation run; 2) the vard utilization rate, expressed in terms of number of containers in the yard over its operative capacity; 3) the quay utilization level, expressed in terms of percentage of utilization of berthing area; 4) the "gang" utilisation rate expressed in terms of percentage of utilisation, i.e. busy time, of the shifts, 6 hours long, involved in the loading and unloading operations of each ship; and 5) the rotation index given by the ratio between the run period considered, i.e. 30 days, and the average dwell time.

Note that apart from the above mentioned indexes many other performance metrics can be used depending on the specific purpose of the scenario analysis performed.

Table 3. CI and CPU for alternative running configurations

,	90%				
n	n Mean (X(n))		Half	Relative	- CPU
			Lenght	Error	
5	37332,800	+/-	378,921	1,015%	2' 18"
10	37391,400	+/-	253,800	0,679%	4' 36"
20	37382,550	+/-	131,072	0,351%	9' 09''
30	37398,767	+/-	114,288	0,306%	12' 21''
40	37398,300	+/-	96,593	0,258%	16' 33''

Moreover, one of the aim of our simulation study is to derive performance indices for evaluating the efficiency of the terminal under consideration; for this reason it is important to choose the conditions under which the performance indexes are computed with an acceptable level of errors (Law, 2007). In this case, we calculate the 90% confidence interval (CI) related to the random variable X, defined as the containers monthly throughput of the system, by making 5, 10, 20, 30, 40 IID replications (Table 3). The independence of replications has been obtained by using different random numbers for each replication. Note that the containers monthly throughput for each replication has been calculated by using the Parts Reports Statistics, provided by Witness. In particular, note that the performance measure herein analysed is the sum of the number of import and export containers that have been shipped out during each replication, one month length. Consequently, the column "Mean X(n)" of Table 3 reports the sample mean of the total containers' throughput calculated in the n=5,10,20,40 replications, respectively. By the comparison of the half length error, we can see that by using 40 replications we are able to reduce its value below the "100 containers" level considered acceptable from the terminal management point of view. Note that to make n=40 IID replications the computational time (CPU) required is about 16 minutes (see Table 3).

CONCLUSIONS AND FURTHER RESEARCH

In this paper, we have presented a discrete event simulation model developed to get some help in the expansion plan of a terminal located in the port of Genoa, Italy. From some preliminary results the proposed model seems to be a useful tool for comparing and analysing different management decisions.

An extensive experimentation is in progress in cooperation with the terminal management. In particular, we are involved in an extensive scenario analysis for evaluating, among others, the growth of the traffic volume, the optimal trade-off between investment required for adding new yard and quay equipments and added value due to larger containers' movements, different operatives rules and handling techniques for the berthing and stacking area, etc. Moreover, a future direction of our research will be to study the integrated use of optimisation and simulation, with the aim of generating optimal solutions to some critical decision problems which can be used as input data for the simulation model. In particular, following the critical factors underlined by the terminal managers, we will firstly approach the Gang Deployment Problem (GDP), that is the problem of determining the amount of resources (gangs) needed to perform the loading and unloading operations of each ship entering the terminal taking into consideration both the overall gang cost and the ship cost related to the time the ship spends on berth. Secondly, we will attempt to provide solutions to the cranes scheduling problem which could generate the gang work plans for each ship entering and leaving the terminal and manage the work sequences on each crane in the terminal with relevant cost savings.

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PRACTICAL ASPECTS OF MODELLING IN THE TRANSPORT NODE RECONSTRUCTION IN RIGA

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KEYWORDS

Decision-making, transport planning, microscopic simulation model, transport node capacity, experimentation.

ABSTRACT

The paper describes the questions of decision support system in transport planning. One of the methods used for studying the relationships and underlying the transportation decision-making is transport modelling, which includes traffic modelling on micro and macro levels. The research considers the example of the microsimulation model of Riga complex transport node. At first, the simulation model for this node using package VISSIM was constructed. This model was based on the real traffic measurements in this area. Further, the two sets of experiments with the model were undertaken: 1 with fulfilled reconstruction and 2 - with offered improving of this node. The data prognosis of this traffic for 8 years was used in both experiments.

INTRODUCTION

Cities have developed over many years and both their transport and their social systems are complex. It is clear that these problems cannot be solved by simply increasing transport supply; demand management is both desirable and necessary. Complexities of city structure, an integrated systems approach to travel, demand management on the base of modelling and simulation provide the best opportunity for the development of equitable, efficient and sustainable urban transport systems (Kabashkin et al. 2003).

Decision-makers have to take into account a large number of factors influencing their decisions and a large number of factors influenced by the decisions. This is especially true in the field of traffic and transport, as transport is dependent on economical developments (growth and spatial organisation of economic activities). As Ginzberg and Stohr's (Ginzberg and Stohr 1982) define Decision support system (DSS) as "...a computerbased information system used by decision-makers to support their decision-making activities in the situations where it is not possible or not desirable to have an automated system perform the entire decision process". The DSS for transport planning helps the user (decisionmaker) to modify the information as needed to define alternatives before he starts the decision process. For implementing the decision support system in transportation the two tasks are important. Firstly, it is necessary to have access to a high-end information system with qualified and full statistical database about the urban movements and the other transport information. The quality of the data models is very important for DSS tasks. The process of these data collection may be organised on the base interview with passengers; the outer observation or traffic statistics obtained with the help of objective control systems on the basis of modern transport telematics aids.

The second task for implementing the decision support system in transportation is the set of realized transport models on macro- and micro-levels. The macroscopic model simulates current and future transport flows, the city road network, analysis of the intensity of movement, scenario 'what if' scheduling. The microscopic model simulates transport jams forecast, chooses the optimal organisation of transport movement on junction, and analyses the "bottlenecks" in the transport network.

The DSS is intended for transportation planners and engineers, transportation researchers, and policymakers. User's input should include transport system operational parameters (roadway characteristics, traffic characteristics, and system operational strategies), transit signal priority alternatives, and stakeholder concerns and preferences. The desired DSS output includes graphic and numeric results relating to economic analysis (payback period, capital recovery period, NPV etc.), operational performance (transit runtime reduction), transit signal priority strategy alternatives etc.

The Riga transport system does not satisfy today's needs of the population for travelling. Considering global character of problems, in plans for development of the city the Riga Council stipulates some ambitious projects: to move an administrative centre from the city centre to the left bank of the Daugava River, in Pardaugava area: to construct the new bridge and to reconstruct wholly the node around this bridge etc. It is expected that the given re-planning will lead to the reduction of congestion of the city centre and will lower the acuteness of the problem of the bridge's capacity. However, such cardinal changes demand the careful analysis of current situation, transport flow forecast and modelling and answering questions "what if". These are the real tasks for decision support system in the city logistics and transportation. In the paper (Kolmakova et al. 2006a) the tasks of decision support system in transportation and city logistics are considered.

The paper includes the example in which the simulation models were used later than it was necessary and the problems that should be really solved were not settled in time.

OBJECT OF INVESTIGATION

The transport interchange "Slavu Street – Krasta Street – Maskavas Street" ("SKM" interchange) with constantly appearing traffic jams was considered to be the object of investigation. The role of this interchange is almost huge because of its disposition: it connects the important ways for freight transportation and provides the way from the bedroom communities to the center of Riga. The scheme of its disposition is presented in Figure 1.



Figure 1: Scheme of the "SKM" Interchange

It earlier attracted the attention (2004) because of its permanent congestion condition. The Transport and Telecommunication Institute (TTI) experts proposed the new design of "SKM" interchange and set up the hypothesis that this decision will improve the current situation. The simulation model with the aim to test this hypothesis was implemented. The given results demonstrated that proposed hypothesis was true and the proposed design doubled the throughput capacity [4]. But the obtained decision remained on paper and was not considered by the government because of starting the new project implementation at that time – the building of the new bridge (South bridge). It will be the biggest bridge in Riga and Latvia which will connect the right and the left Riga banks of Daugava. The considered interchange falls under the reconstruction within the borders of this project. According to this project the "SKM" interchange will be the connecting link between the South Bridge and the railway Slavu Bridge and it was planned to be reconstructed as a threelevel flyover. However, this project was developed on the base of the experts' estimation and engineering solutions only. The simulation approach was not used at the stage of this interchanges and new bridge designing. The TTI researchers decided to try to estimate the future situation when the bridge will be put into commission.

The main goal of the investigation was to make the comparative analysis of the considered interchange throughput capacity as it was in 2004 and as it will be in 2012, when the project will be done. As the base for the analysis the results of the implemented project in 2004 were considered (Kolmakova et al. 2006b.). Also, the simulation model of the new trestle design was implemented taking into account the future traffic properties.

As an instrument for simulation model implementation the package VISSIM 5.1 family PTV Vision has been selected. At first, the simulation model for this node using package VISSIM was constructed. This model was based on the real traffic measurements in this area and the forecast data of traffic volume in 2012. The traffic characteristics of the renovated transport node are investigated and compared to the traffic characteristics of this node in 2004. It is necessary to estimate the capacity of the existing transport node from the point of view of today's situation and possible increase of the intensity of vehicles travelling in the future (in 2012).

CONSTRUCTION OF THE MODELS

One of the starting conditions of an adequate model creation in VISSIM is the presence, at least, of one scaled map displaying a true network. Due to such opportunity in the package, the model approximates reality as much as possible. On the basis of the map proposed by the architectural agency of LTD "TiltProjects" in the format of AutoCAD and the information on the forecast of the transport flows intensity, their description and distribution along the network supplied by the LTD "*imink*" (Niedole et al. 2005) the simulation model of the analysed area has been constructed.

The data on intensity and traffic volumes were forecast for the summer period of 2012 (8:00 - 9:00). The screenshot of simulated transport node with 5 areas, being sources of traffic, is presented in Figure 2.

Standard VISSIM types of transport (Car, HGV, Bus, Tram, Bike, Pedestrian) are used as objects of the model. The set of options was defined for each type (length, acceleration and deceleration functions etc). The traffic composition (proportion of Cars, Buses and HGVs) is presented in Table 1.

Transport units' routing has been set in the form of static O/D ways where it has been necessary to set the simulation time and the relative flow of vehicles for the

chosen network area. The volumes of traffic flow from 5 sources divided by 3 main modes are presented in the Table 2. OD matrixes for 2004 and 2012 years are presented in Tables 3 and 4 respectively.





	Type of vehicle		
Traffic Source	Car	Bus	HGV
Krasta	87%	2%	11%
Maskavas (Centre)	92%	0%	8%
Maskavas (Rumbula)	90%	3%	7%
Slavu bridge	90%	1%	9%
South bridge (2012.g.)	90%	1%	9%

Table 1: Traffic Composition for 2004 and 2012

 Table 2: Amount of Vehicles per Hour for Every Area

 Generating an Input Stream

Traffic Source	Year	Car	Bus	HGV	Total
South	2004	0	0	0	0
Bridge	2012	3406	55	320	3780
Maskavas	2004	1922	68	140	2130
(Rumbula)	2012	2774	98	202	3074
Maskawas	2004	53	0	4	57
(Centre)	2012	77	0	6	83
Slavu	2004	1174	19	110	1303
Bridge	2012	3153	51	296	3500
	2004	1928	35	250	2213
Krasta	2012	1759	32	228	2020

Numerical characteristics of implemented model complexity:

- simulation model was constructed from 465 fragments (type of object in VISSIM -«Link&Connector») on the basis of the map given by the architectural agency of SIA "TiltProjects" [5];
- 20 points of traffic sources were introduced to the model, 13 of them being the sources of vehicle flow and 7 of them the sources of pedestrians and bike flow;
- 68 decision points were described in the model;
- 7 priority rules were introduced and 49 conflicted zones were defined;
- 3 groups of traffic lights were described;
- main speed at intersection 50 km/h and few zones with the speed of 70 km/h were introduced.
 32 Desired Speed Decisions objects were introduced;
- Data Collection Points 36, Queue Counters -17.

	Maskavas (Rumbula)	Maskavas (centre)	Slavu bridge	Krasta
Maskavas (Rumbula)	-	31%	42%	26%
Maskavas (centre)	-	-	-	100%
Slavu bridge	-	3%	-	97%
Krasta	23%	30%	46%	-

Table 3: OD Matrix (in %) in 2004

Table 4: OD Matrix (in %) in 2012

	Maskavas (Rumbula)	South bridge	Slavu bridge	Krasta
Maskavas (Rumbula)	-	31%	7%	63%
South bridge	4%	-	85%	11%
Slavu bridge	0.1%	31.2%	-	68.8%
Krasta	73%	3%	24%	-

During the experimentation the model parameters have been varied to make the intensity and structure of transport flows correspond to the observable ones – thus the validation and calibration of the model has been made. To validate the model the distribution of the total volume to the single lines was examined. The method of "Significant Intervals" was used for validation. The results demonstrated that the models are trustworthy.

EXPERIMENTATION WITH THE MODEL AND COMPARATIVE ANALYSIS OF SIMULATION RESULTS

Three experimentation plans were performed during the investigation:

- 1. experimentation with the SKM crossroad as it took place in 2004;
- 2. new "SKM" interchange throughput capacity investigation taking into account the traffic flow forecast for 2012;
- 3. investigation of the efficiency of the proposed decision which was aimed at decreasing the negative influence of the non-optimal organization of one of the crossroads.

The key differences between the first two experiments are architectural decisions on the organization of the transport node, distinctions in the volumes of traffic and distribution of stream to directions. Every experiment included 50 runs of simulation model, every run was imitated by the hour of work of the real system.

The following measures were considered:

- Average time of some section crossing per vehicle, s.
- Average delay time per vehicle, s. Delay time subtracting the theoretical travel time from real travel time; it doesn't include passengers' and transit stops.
- Average stop delay per vehicle, s. it does not include passengers' stop times at transit stops or in the parking lots.
- Average stops number per vehicle, not including stops at transit stops or in parking lots.
- Total time the vehicle spent in congestion, s.
- Average, maximum queue length (m), number of vehicle stops within the queue.

Some of these measures are presented in Table 5.

The results demonstrate that the proposed new design on transport node SKM will increase its throughput capacity. The average speed will be increased by 19%, the average vehicle stop delay will be decreased by 46%. But the particular analysis of the several fragments of the interchange demonstrates that the throughput capacity improving has the fragmentary nature.

Several crossroads of this interchange were studied. As the criteria of the consideration was used the index of the level of service (LOS). It is the description of the level of the transport node' workload that was realized in the package of VISSIM, and settles accounts on the basis of delay time on the intersection. The delay time was evaluated as a difference between the time, which was spent by the vehicle in crossing of the intersection and the time, which would be spent by the vehicle at a free stream. A delay does not take into account the delay time because of the signal of the traffic light.

The results demonstrated that the majority of crossroads had normal LOS, except the crossroads Maskavas 1 (N1), Maskavas 2 (N2), Krasta-Maskvas (N3) (Figure 3). The LOS indices of interchanges N1 and N3 were in

2004 really high, equal to F (last legitimate value LOS equal to D) and for N1 equal to D.

Table 5: Measured Results of the Experimentation	with
the Model	

Measures	Year	Average	Standard deviation	95% signif.level	Min	Max
lelay hicle, s	2004	103.9	2.0	104.7	100.6	107.9
Average time per ve	2012	85.5	1.5	86.0	82.7	89.2
e num. s per cle	2004	11.6	0.4	11.7	10.7	40176
Average of stop vehi	2012	10.5	0.5	10.6	10	11
Average speed, km/hour	2004	13.6	0.2	13.70	13.3	13.9
	2012	29.9	0.3	30.0	29.6	30.5
Average stop delay per vehicle, s	2004	56.3	1.8	20821	53.8	59.2
	2012	30.4	0.4	30.6	29.6	31.4

It is possible to notice that in spite of the fact that intensity of traffic to 2012 grew on the whole, the reconstruction of this transport node allowed improving the LOS on the areas of segments N3 and N1; however, the level of service on segment N2 remained unsatisfactory (F).



Figure 3: Layout of Transport Node with the Problem Zones

Comparison of the state of three problem zones for the purpose of vehicles delay makes it is possible to mark the change in architecture of this transport node, intensity of traffic and redistribution of streams resulted in diminishing of temporal delay on the segment N1 and N3, but did not have a positive influence on the segment N2. The mean delay time in this area for 2012 will even grow by 10% (Figure 4).



Figure 4: Average Delay Time in the Problem Zones for 2004 and 2012

The reason for this situation is the pedestrians' light signal disposition in this area. The hypothesis was proposed that the excluding of this light signal (it is possible because of building the pedestrians' subway) will reduce the level of saturation in this transport system segment. This hypothesis was tested by the simulation of the new model without the pedestrians' light signal was implemented and 50 experiments with it were carried out. The experimental results demonstrated that the proposed reconstruction will be helpful and resolve the existing problem. The comparative characteristics are presented in Table 6.

The average speed increased by 34%; the average delay time decreased by 53%. The LOS of the interchange segment N2 changed from the level F to the level A (the best level of service).

Also the level of air pollution in this segment was considered; that is why the traffic jam involves the increasing of emission and as a result the pollution of the air. The level of CO, NO_X and VOC was measured. The comparative analysis demonstrated that the level of the pollution decreased by 18%; that undoubtedly will have a good influence on the ecological situation.

The 3D film which may be used for the presentation of new project as well as the tool for making decision of existing problem solution finding was made. The example of the 3D model is presented in Figure 5.

Table 6: Measured Results of the Experimentat	tion	with
the Reconstructed Model		

Measures	Experiment	Average	Std.Dev.	95% Signif. level	Minimum	Maximum
Average speed,	2-nd	29.96	0.25	29.98	29.55	30.47
(km/h)	3-rd	40.08	0.33	40.13	39.37	40.76
Average	2-nd	85.49	1.48	86.02	82.74	89.2
delay, (s)	3-rd	40.24	1.13	40.59	37.79	43
Average number of	2-nd	10.52	0.50	10.63	10	11
stops	3-rd	1.96	0.20	2.02	1	2
Average stop delay,	2-nd	30.38	0.35	30.59	29.63	31.36
(s) (s)	3-rd	8.51	0.22	8.93	8.04	9.1



Figure 5: View on the Three-level Flyover in 3D Animation

CONCLUSIONS

During the investigation there were implemented several simulation models of Riga interchange: the model of the old design of crossroad, two models of its new designs, and the model which was aimed to resolve the existing problem of the new design made by the planner. The obtained simulation results quantitatively demonstrated the level of the proposed service by the old crossroad, new crossroad design and allowed proving the expediency of the proposed way of solving the existing problem.

The results of carried on investigation rigorously prove the necessity of the application of the simulation at all stages of the transport system evolution. The obtained results demonstrated that the timely applied simulation may resolve the current crossroad problem on the stage of its designing and may reduce the expenditure for removing it now.

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Simulation of Complex Systems

TORSIONAL MODEL AND ANALYTICAL SIMULATION FOR COMPLEX ROTATING MACHINES

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KEYWORDS

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ABSTRACT

Complex rotating machine trains especially trains including electric machines are subject to the most varied and often most severe torsional disturbances. If shaft or rotating component failures occur as a result of torsional oscillations, the consequences can be catastrophic. In this paper a comprehensive model and simulation method using analytical formulations are developed to study both steady state and transient response of complex rotating machine trains including several machines. Analytical results are presented and recommendations for torsional reliable trains are addressed. Couplings being the more accessible components within the train are often modified to tune the overall system. Recommendations for coupling are: High torsional stiffness coupling (best and optimum option, if torsional simulation confirmed frequency separation and transient torques) or flexible coupling (more elasticity and damping and more maintenance) or integral rigid forged flange connection (more rigidity, high natural frequencies and much less damping).

INTRODUCTION

Complex rotating machine trains are now a day becoming common trains in petroleum, petrochemical and chemical industries (Bloch 2006). An example is train including compressor, electric motor driver and turbo expander gas recovery turbine for efficient operation (three machine casings, compressor - motor recover turbine coupled through couplings and clutch). Complex rotating machine trains are consisting several rotors, shaft intervals and machine casings including drivers, rotating machines, electrical equipment and recovery turbines. The expected level of reliability and availability of rotating machine train in petroleum and chemical industries, is very high and it presents a real challenge to machine designers and operators. Advanced methods shall be applied in order to obtain the highest level of safety and reliability.

Complex rotating machine trains have complicate tosional behavior. These trains have several complex shafts and rotors, electric machine rotor(s), couplings and relatively flexible shaft extensions. They may also include flywheel, gear unit(s), clutches (such as SSS –

Synchro Self Shifting Clutch) or turbo expander turbine in special cases. Electric machines can introduce operational problems from electrical events that produce pulsating torques. Also rotating machines can introduce mechanical torsional excitation torques. When used in trains, since connected machines function as spring systems in series, the potentials exit for torsional resonance and torsional fatigue damage.

If shaft, rotor or rotating component failures occur on rotating machine train as a result of shaft or rotor torsional oscillations, the consequences can be catastrophic. An entire train can be wrecked as a result of the large unbalancing forces that can arise following shaft separation. These have actually occurred (Walker 2004). There is also potential for vast damage and loss of human life. For these reasons great attention is generally taken to ensure that rotating machine trains have the required torsional capacity. In this paper a comprehensive model and simulation method using analytical formulation are developed to study both steady state and transient response of complex rotating machine trains.

TORSIONAL MODEL OF TRAIN

Torsional vibration involves angular oscillation of the rotors of machines. Each rotor or shaft in the system will oscillate following a torsional disturbance to the train. The design of train shall include optimization for dynamic loads acting on foundation, unbalance forces, shaking forces, irregularity degree and torsional stresses. All these factors need detailed torsional analysis to ensure proper design and reliability. The torsional behavior is key determinant of reliable operation of train. It is vital for ensuring reliable machine operation due to machine stimuli that range from rarely occurring high level transients to continuous relatively low levels of excitation. Correct application of torsional analysis practices and improved transmission system design and operating practices can generally rendered train robust to the effects of stimuli from different sources. These events can be from the electrical transmission network, or mechanical equipment malfunction, or from problems within the electric machine (such as short circuits or faults), or mechanical rotating equipment problem, or fault in electrical system, or other mechanical or process sources to which the train is connected (such as transformer, process plant, etc).

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It is of paramount importance to avoid torsional resonance (particularly at or near the lower harmonics of train operating speed frequency), and to ensure that shafts and other components are suitably sized to avoid failure or significant damage during possible sever transient disturbances. The procedure for torsoinal analysis and simulation include following steps. Modeling of train, calculation of undamped natural frequencies, harmonic components calculation and forced vibration calculation.

The model must be accurate enough to simulate the real system behavior at least for frequencies below the 20th multiple of the maximum rotating speed. Only a model with enough details and large number of elements make it possible to evaluate higher number of vibration modes. In the other hand very high frequency additional modes (such as frequencies more than 20th multiple of the maximum rotating speed) has no effect since no resonance is foreseen and they are related to low amplitude exciting harmonics (Giacomelli et al. 2006).

Basically the model is represented by a number of rotating masses connected to each other by means of mass-less shaft intervals with appropriate torsional stiffnesses. Rotating masses can represent both the rotor or shaft intervals and the connected components to each interval. The mass elastic model of rotor or shaft is created by lumping the inertia. Generally rotor or shaft between two bearings can be modeled as single masselastic element. However for complicated and complex intervals which include many details and components more sophidticated model including several mass-elastic element shall be used. The coupling is modeled as a single torsional spring (coupling sub-vendor supplied torsional stiffness) with the inertia of the associated coupling halves at each end. These inertias are added to the rotating machine shaft model masses in both sides of coupling. Proper dedicated lumped masses for all accessories (such as flywheel, gear wheel, exciter, connecting flange, etc) shall also be added to model. Model and formulation parameters are as follows:

 θ_i Torsional displacement of mass *i* (rad).

- J_i Polar moment of inertia of mass *i* (kg s³/m).
- K_i Torsional stiffness of the shaft internal *i* (N m).
- C_i
- Damping coefficient for interval *i* (kg s²/m). Damping coefficient for the mass *i* (kg s²/m).
- C_{Mi} Model lumped mass total number. п
- т Maximum machine torque harmonic order.
- Torsional natural frequency (rad/s). ω
- M_i Applied torque to mass *i* (N m).

NATURAL FREQUENCIES OF TRAIN

The next step is calculation of the train undamped torsional natural frequencies. The goal is to locate natural frequencies away (usually by 10%) from potential excitation frequencies that might come from both the rotating and electric machines (Rangwala 2006; Brown 2005). In addition, it is recommended that natural frequencies be placed 10% outside of electrical net frequency and 5% outside of its second multiple (Walker 2004). Natural torional frequencies reach

higher values as their order increases and in practice the first three modes of vibration usually need to be investigated in detail.

Torsional natural frequencies come from solution of Equations (1). The calculation of the undamped natural frequencies is a problem of eigenvalues and eigenvectors which represent natural frequencies and mode shapes respectively.

$$J_{1}\ddot{\theta}_{1} + K_{1}(\theta_{1} - \theta_{2}) = 0$$

$$J_{i}\ddot{\theta}_{i} + K_{i-1}(\theta_{i} - \theta_{i-1}) + K_{i}(\theta_{i} - \theta_{i+1}) = 0 , \quad i = 2,...,n-1 \quad (1)$$

$$J_{n}\ddot{\theta}_{n} + K_{n-1}(\theta_{n} - \theta_{n-1}) = 0$$

Generally most rotating equipment and electrical machine have a low level of torsional damping (Walker 2004; Giacomelli et al. 2006). It is found that the amount of torsional damping in turbomachinery is very low unless special provisions are made. For heavy duty machines, it is impractical and uneconomical to employ mechanical damping devices to substantially reduced peak vibration response levels following severe torsional vibration (Walker 2004). Because of low damping level, undamped natural frequencies can represent natural frequencies of real train (Giacomelli et al. 2006). Observations are in agreement with this assumption. The torsional mechanical response will generally be multimodal with a slow decay rate because of the light damping (Walker 2004; Giacomelli et al. 2006)

The main concern is for first torsional natural frequency position because higher natural frequency orders are associated with high harmonics which have little effects. In case the torsional natural frequencies do not meet mentioned margins (10% away from potential excitation frequencies), individual train component can be modified. Parametric study of presented natural frequency calculation method can provide information on how to tune rotating machines train, if natural frequency separation margins are discovered to be unacceptable for reliable performance. Modification of coupling torsional stiffness by an appropriate tuning of the coupling type or space diameter is primary and easiest solution. Generally the coupling is the most flexible shaft interval in train and has a strong influence on first torsional natural frequency. Range of available coupling options is vast. From flexible coupling to rigid forged flanged connection (without coupling). However If coupling modification is not sufficient and further modification is required (mainly in case of more torsional stiffness required to raise first torsional natural frequency) modification of electric machine shaft geometry (mostly diameter) can be studied jointly with electric machine sub-vendor. The modification of rotating machine (process critical compressor, heavy duty steam or gas turbine, etc) rotor or crankshaft geometry is very difficult and in most cases it is never modified to accommodate torsional application requirements.

DAMPED STEADY STATE TORSIONAL RESPONSE

If there is interference between torsional natural frequencies and excitation harmonics and modification is not desired or possible, it is necessary to make torsional stress analysis. Stress analysis shall be performed to ensure that the resonance will not be harmful for the train. First step is steady state torsional analysis. The analysis should be performed for all possible operating conditions including all possible speeds and capacities. The governing equations of system to calculate the damped forced torsional vibration are as Equation (2).

$$J_{1}\ddot{\theta}_{1} + K_{1}(\theta_{1} - \theta_{2}) + C_{1}(\dot{\theta}_{1} - \dot{\theta}_{2}) + C_{M1}\dot{\theta}_{1} = M_{1}$$

$$J_{i}\ddot{\theta}_{i} + K_{i-1}(\theta_{i} - \theta_{i-1}) + K_{i}(\theta_{i} - \theta_{i+1}) + C_{i-1}(\dot{\theta}_{i} - \dot{\theta}_{i-1})$$

$$+ C_{i}(\dot{\theta}_{i} - \dot{\theta}_{i+1}) + C_{Mi}\dot{\theta}_{i} = M_{i} , \quad i = 2,...,n-1$$

$$(2)$$

$$J_{n}\ddot{\theta}_{n} + K_{n-1}(\theta_{n} - \theta_{n-1}) + C_{n-1}(\dot{\theta}_{n} - \dot{\theta}_{n-1}) + C_{Mn}\dot{\theta}_{n} = M_{n}$$

The general expression of the steady state applied torques (M_i) includes a vibrating component superimposed on an average torque level as per Equation (3). Train load torques can be decomposed, through a "Fourier" analysis, into series of sinusoidal curves which frequencies are multiple of machine running speed and modulus generally decreases as the harmonic order increases. The higher the number of harmonics considered, the closer the results to real torque. Optimum solution suggested as calculation of 25 harmonics (m=1 to 25).

$$M_{i} = \sum_{p=0}^{m} M_{i,p} \sin(p \omega t + \alpha_{p})$$
(3)

The torsional dampening is assumed to be the hysteretic (Harris and Allan 2002; Giacomelli et al. 2006). Each applied torque must be properly phased with respect to relatively train rotor angular position. The electric machine torque supposed to be constant during steady state load however there are relatively small fluctuating torques components due to interactions between the current pulsation of electrical elements (such as winding) and electrical machine shaft mechanical irregularity degree. These fluctuations generally can be neglected for steady state response. Solution of Equation (2) can be obtained based on "Principle of Linear Superposition". The system is composed of (n)linear differential equations with (n) parameters, tridiagonal and symmetrical. Its solution can be transferred to the solution of (m) differential equation system (each equation related to different harmonic of the exciting forces).

A sensitively analysis should be always carried out to take into account all possible variances affecting the model especially those due to fluctuations of running speed (such as net frequencies, etc) which can shift the harmonics of the running speed. Variations of the mass elastic data (i.e. coupling stiffness, rotor inertia, etc) can shift the torsional natural frequencies. Alternative option of considering the relative position of the harmonics and natural frequencies, is to calculate the torques and stresses over a range of 10% of the rated speed. The highest values within that range can be comparable to correspondence endurance limit for torsional fatigue. For a train, torsional stress is function of related position of torsional natural frequencies and exciting harmonics.

TRANSIENT TORSIONAL RESPONSE

There are usually many cases of transient disturbances which should be modeled. The transient torsional analysis requires a different and more time consuming calculation method since it requires a direct integration of the motion equations. In this case the solution is time dependent.

The differential equations of motions are similar to those of the steady state as Equation (2), but they have different exciting torques. In this case rotating machine torques (M_i) components shall be obtained. Inertia and fluid transient torque components shall be separately calculated. Train speed variations affect the inertia transient torque components and fluid transient torque contributions in different manner. For some rotating machines (such as positive displacement machines) fluid transient torque components can be assumed without considerable changes when speed changes. However electric machine torque excitation is not periodic. As result, in general, train transient torque excitations can not be given in "Fourier Series". The transient analysis out put is generally represents by torque and stress plots for each rotor as a function of time. However the main results of the transient analysis can be given in terms of peak shear stress in machines and peak torque on couplings.

The highest stress / torque amplitudes acting on rotating equipment, electric machine and coupling shall be compared to the endurance limits of each of the respective components. In case the torques and stresses are not within the allowable endurance limits, a redesign must be carried out in order to achieve a wider separation margin between torsional natural vibration frequencies and high amplitude harmonics to obtain lower stresses.

The fact that the damping of the train is low can lead to the generation of extremely high transient torques in train shafts as a result of response compounding if torsional disturbances occur in rapid succession.

The resulted alternating stresses in the train shafts and other components need to be below the fatigue endurance limit of the material involved. This is because of the very high number of stress cycles that will be experienced over the life of the machine as the cycles are being accumulated continuously.

ELECTRICAL EFFECTS ON COMPLEX TRAIN

It is most important to study problems from electrical events that can produce pulsating torques and torsional vibration in complex rotating machine train. There are wide varieties of incidents that can cause electrical current oscillations in the electrical transmission to which the electric machine is connected. In each case, the incident results in an oscillating torque applied to the train, which can stimulate twisting oscillations in the machine shafts and vibration of various rotating and non rotating components.

Electrical transient disturbance can be planned or unplanned (emergency) transmission line switch incidence, electrical faults in the transmission network such as electrical circuit breaker actions or fault caused by storms, electric machine internal faults or terminal short circuits. In case of power generation (rotating machine coupled to electric generator) transient disturbance can be mal-synchronization of the generator to the electrical network. These transient oscillations generally include a step change in torque (impulse) and discrete frequency torque components at the first or second harmonics of the power system frequency, with generally low levels at the higher harmonics. The step change torque component decays quite slowly (order of seconds) however the lower harmonics of the power system frequency decay rapidly in comparison (order of tenth of seconds).

An example of this is with the use of some forms of high speed reclosing of electric transmission line circuit breakers following the electrical faults in network. As discussed electrical line fault can result from either temporary or permanent electrical transients (for example electrical lighting strike, transmission line break, a tree fall into a transmission line causing long term transmission line phase to phase or phase to ground fault, etc.). Following any type of electrical fault in the transmission line with one form of high speed reclosing, the power circuit breakers automatically open after a few electrical cycles (1/50 of seconds) to isolate the fault and then automatically reclose after only several tenths of second. If the fault has cleared during this period then no significant shaft torque compound occurs. However high percentage of severe multiphase faults are permanent and thus may not benefit from high speed reclosing. In case of permanent fault then a second major torsional event will be experienced by the magnitude approximately equal to that of the first one. As the damping of the torsional modes is very light the response amplitudes in the shafts from the first electrical disturbance will be decayed only slightly when the circuit breakers reclose into the fault for the second time. If the timing of this reclosure is at its most unfavorable, the shaft torques could approximately double as a result of response compounding.

There is potential for torsional insatiability on trains connected to electrical networks that have series capacitor compensated lines to reduce power transmission losses (sub-synchronous resonance or SSR). Machines connected to direct current transmission lines can also be affected with instability in this case due, for example, to incorrect operation or mal-adjustment of rectifier and inverter control equipment. In such these cases, torque pulsations are produced by electric machine due to current pulsation and magnetic fields interactions. In general these torque pulsations do not cause any harm unless their frequency (resistance, inductance and capacitance circuit introduces an electrical resonance frequency) coincides with, or is close to, one of the torsoinal natural frequencies of the train. Under these conditions the shaft response torque could build up to extremely high level.

Recommended corrective actions for SSR problem included installation of large filters to remove the harmful current frequency components from entering the electric machine, installing electrical damping devices, and addition of protective monitoring and relaying equipment (Walker 2004).

The rectifiers, inverters, high voltage direct current (HVDC) transmission system or large nonlinear electrical systems feed significant harmonics of the fundamental power frequency into electrical network. Train is subjected to significant high order harmonic currents entering the armature of the electric machine which produce pulsating torques on the rotor, causing torsional vibration. These pulsating torques are at (6n) harmonic frequencies (6, 12, 18, etc) and would be of concern only if they become resonant with a train torsional natural frequencies. The lowest harmonic torque frequency and the one that generally has the highest amplitude is the sixth harmonic. Higher order harmonic torques are therefore rarely of concern (Walker 2004).

Certain harmonic effects arise when an electric machine is started. Usually the main concern is with torque dips in induction motors, which affect motor's ability to reach full speed. But there are some effects that can result in torque pulsations. These are due to interactions between various sources of harmonics in machine magnetomotive forces and fluxes. The main sources of harmonics are distribution nature of the stator winding, distribution nature of rotor currents, slotting on the stator (or rotor) which produces a permanent variation at slot pitch frequency and pulsation of main flux because the average permeance of the air gap fluctuates as the rotor moves relative to the stator. The interaction between all these different harmonic sources can produce torques that rise and fall with speed, sometimes accelerating the shaft, sometimes slowing down the shaft. Torque pulsation frequency will vary as the machine speed changes. These torques and their magnitudes depend on the relative number of stator and rotor slots, the use of open and closed slots, the rotor slot skew, and the electric machine reactance and resistances. There have been reported cases (Walker 2004) of torques large enough to cause damages.

IRREGULARITY IN COMPLEX TRAINS

For some rotating machine trains (such as reciprocating trains), flywheel is mandatory to regulate variable train torques. Irregularity degree for mechanical component reliable operation is maximum 2%. This value is minimum requirement for all trains. Generally in accordance with specific requirements of electric

network, electric machine (especially current pulsation), rotating equipment, operation, torsional vibration results, train complexity, etc, lower irregularity value is required. It is recommended to obtain 1% for special purpose units in petroleum and petrochemical plants. Irregularity values between 1-1.5% are in common use.

VARIABLE SPEED COMPLEX TRAINS

Variable frequency motor drives are becoming more popular (Brown 2005). For variable speed multimachine rotating equipment trains, complex issues of torsional response and feedback due to torque pulsation shall be addressed.

Because of the complexity of the train, the system is limited in its turn down by torsional problems. Torsional analysis is vital for development of relatively new technology of variable speed multi-machine complex trains. In variable frequency drive (VFD), the inverter converts the AC power to a series of DC voltages, and then varies the frequency of DC pulses to approximate a sinusoidal waveform at the desired frequency. The AC waveform produced by this process is rich in harmonics because the fast switching creates voltage spikes. This results high order harmonic torques to electric machine and consequently to complex train. During normal and transient operation and the frequency run up and run down, there are large number of potential operating speeds and hold points. There are significant risks of the development of resonant mechanical response and mechanical damage. It is important that torsional natural frequencies being calculated and modified as required to avoid resonances. In addition operational strategies include rapid acceleration through defined critical speeds and avoidance of operating hold points near critical speeds shall be carefully respected. Due to wide operating speed range, maintaining 10% margins between all possible excitation frequencies and natural frequencies is very difficult and usually impossible. For variable speed drives comprehensive torsional and stress analysis is necessary.

Torque harmonics generated by variable speed drive can excite the resonance during start up, and therefore must be evaluated. In addition the ramp rate or frequency at which the variable speed drive controls the speed of the units should not coincide with torsional natural frequencies.

A variable speed train may have several damaging torsional resonances within the operating speed ranges due to the machine excitation harmonics intersecting the first torsional natural frequency. With the use of soft coupling, the first tosional natural frequency can be tuned below minimum speed. In many instances this is the only way to achieve the full desired speed range. Otherwise the speed range has to be limited or certain speed bands have to be avoided.

Soft coupling in variable speed train can add damping to the system. However dynamic torque should be calculated and compare with coupling limits. In addition limited soft coupling life can be a problem. High torsional stiffness coupling can reduce maintenance but large portion of speed range may be avoided. Comprehensive torsional analysis and study must be used to obtain optimum solution.

SIMULATION RESULTS

Analytical results are presented for a multi-throw complex (four throws and three cylinders) heavy duty reciprocating compressor coupled to electric motor driver (direct coupled eighteen (18) poles 6.5 MW induction electric motor) with variable frequency drive VSD for start up when plant is in isolated situation (disconnected from country electrical network). Four step capacity control, 0-50-75-100%, using fixed volume pocket at cylinder head end and suction valve unloaders are provided. Available coupling options are: High torsional stiffness coupling (if allowed by torsional analysis), flexible coupling or integral rigid forged flange connection with single bearing electric machine. Extensive simulations show for this train regarding natural frequency interfaces and all possible transient cases, flexible coupling is acceptable option due to more elasticity and damping effects which help to obtain acceptable frequency margins and reduce transient stresses. The fist torsional natural frequency of machine is more than seven times the train speed. This implies an adequate separation with respect to compressor exciting harmonics. Simulations show a coupling stiffness variance of about 35% would be required for the train to reach resonance.

Compressor train integrity must be assessed during a three phase short circuit of the electric motor. The transient event assumed to last about 0.5 seconds. In this case the electric motor is subjected to a high frequency and high amplitude oscillating torque. Motor peak torque is around 3 times the normal value. Simulations show that torsional transient response is strongly reduced by train damping from flexible coupling selection. The peak torques and stresses are about 1.5 times their average values.

Start up transient analysis is performed to obtain transient stresses during the train start up. The focus is on most critical intervals including coupling and electric machine rotor. Compressor is started unloaded and the nominal running speed is achieved within 5 seconds. Simulations show electric machine has a high frequency response at the early stage of train start. The peak stresses do not reach significant amplitudes. A local amplification occurs several second after start when the electric machine variable frequency pulsating component crosses the first torsional natural frequency. Properly accounting for abrupt diameter changes in shaft and rotors in train are important due to it can decrease stress concentration and result better system fatigue life.

Figure (1) shows reciprocating compressor brake torque vs. crank angel for one revolution of crankshaft in steady state conditions. Compressor brake torques are dimensionless by rated electric motor torque. The solid and dashed-dotted curves represent compressor torque

for normal full load (full rated flow) and (50%) unloaded conditions (1/2 rated flow) respspectively. This figure shows how compressor brake torque varies considerably in one shaft revolution (from less than 20% of motor rated torque to around 170% of motor rated torque). It shows importance of flywheel to regulate train torque requirements and strong effects of torsional irregular torques on train torsional behavior. Different unloaded conditions show completely different torsional loading behavior. Simulations show unloaded (50%) condition represents highest irregularity in train among steady state conditions. It proves necessity to evaluate torsional behavior of all operating conditions and possible process changes. All torsional transient responses to shift from one operating condition to other shall also be modeled and analyzed.



Figure 1: Reciprocating Machine Brake Torque vs. Crank Angel.

COUPLING SELECTION FOR COMPLEX TRAINS

Many operators and vendors prefer high torsional stiffness coupling because it results to more rugged train and higher natural frequencies. Also it decreases maintenance. The soft couplings can protect the machine components by absorbing the dynamic torque generated by electrical or mechanical events. Rubber coupling usually increase maintenance since the rubber degrades over the time due to heat and environmental factors. Actual rubber coupling life may be significantly less than coupling manufacture stated life, especially if the coupling is subject to heat or harsh condition (such as oil mist, ozone, etc). Special silicon block may improve life for high temperature applications.

For coupling an appropriate service factor should be used to allow for possible transient conditions. The vibratory torque and heat dissipation must be reviewed carefully. The heat dissipation is a function of the vibratory torque and frequency and is normally specified in terms of power loss (Watts). Other factors such as end float and allowable misalignment should also be addressed. The torsional stiffness of the rubber elements can vary with temperature and torque. The actual coupling stiffness can vary by as much as 20% from catalogue values. It shows importance of sensitivity analysis especially for coupling stiffness. Also some coupling (such as coupling with rubber elements) have nonlinear stiffness which depends upon the actual transmitted torque. As system starts, the speed increase can result in a load change and consequently some of the natural frequencies will change (coupling stiffness can change and cause natural frequencies to slightly change). In these cases coupling are usually modeled linear and special attention is required for elastic data sensitivity analysis.

Comprehensive torsional analysis and study, machine arrangement, all possible steady state and transient conditions, operation and maintenance must be considered for optimum coupling selection. In the other words, coupling shall be selected very carefully and with respect to torsional analysis, train arrangement and complexity, operating conditions, foreseen transient conditions and previous experiences.

ELECTRIC MACHINE CONSIDERATIONS

Experiences have shown that only accurate modeling and simulations of electrical machine can result to accurate torsional analysis of train. Observations show that natural frequencies of trains are sensitive to electric machine model. Flexibility and inertial distribution through the electric machine core shall be modeled accurately otherwise it can result in missed torsioal natural frequencies, inaccurate torsional analysis and torsional problems. Stiffness of electric machine shaft can be influenced by the various types of construction. Machined or welded webs can add significant stiffness (typically 10-40% more) while keyed or laminations typically add minimum stiffness. Only a detailed Finite Element Analysis (F.E.A.) of the electric machine shaft can provide accurate results. Comparisons showed more than 30% error in shaft stiffness between detailed Finite Element Analysis (F.E.A.) and simplified method (Feese and Hill 2001).

Experiences have shown that some electric machines have not been designed to couple to heavy duty rotating equipment and may not be adequately sized for heavy duty complex rotating machine trains. An indication can be shaft size. Rotating machine shafts or rotors are often constructed with higher strength material and have lower strength concentration factors. As rule-of-thumb electric machine shaft diameter to be equal to or greater than the rotating machine shaft or rotor diameter.

PRACTICAL RECOMMENDATIONS FOR COMPLEX TRAINS

Numerous torsional vibration problems continue to occur in complex rotating machine trains. Main reasons are lack of comprehensive torsional vibration analysis and study, improper application and maintenance of coupling (mainly flexible couplings) and lack of monitoring. Shaft and rotor materials should be high strength steel. If welds are required on shaft, a weldable shaft material should be used. Proper weld procedures and material compatibility must be considered. Fabrication details (such as the electric machine pole bolt torque, etc.) should consider loads due to torsional vibration. Continuous operation at torsional resonance shall be avoided. Coupling and electric machine torsional characteristics have strong influence on train torsional vibration and can be modified to tune system. Some vendors intended to use stiff system with short flanged connection (no coupling) and single bearing electric machine. These trains have much lower damping however higher natural frequencies. These trains may be acceptable after careful review of torsional analysis including all possible operating steady state and transient torsional situations. It is important to measure and verify torsional vibration during Based performance test. on site observations. synchronous electric machine start up and short circuit cases are critical and shall be respected in details. A train which passes through a torsional natural frequency during start up may produce significant transient shaft stresses. If the system is started on a frequency basis, a start up analysis should be performed to determine if low cycle fatigue is a potential problem. As noted synchronous machines need more care for torsional analysis and they definitely need a transient torsional start up analysis. Coupling torque is usually chosen on the basis of mean requirements for full load. It must have a sufficient service factor to handle and likely overload (such as electrical faults).

CONCLUSION

A comprehensive model and simulation method using analytical formulations are developed to study both steady state and transient response of complex rotating machine trains. The torsional vibration analysis report shall include data used in mass elastic model, torsional natural frequencies, torsional critical speed, mode shape diagrams, interface diagrams, definition of coincidence of the excitation frequencies with the torsional natural frequencies, all possible steady state, all possible transient cases (start up, shut down cases, short circuit, electrical faults, etc), non ideal cases, worst case design, dynamic torsional stresses (based on dynamic torque modulations, stress concentration factors, and amplification factors), comparison to determine compliance (with regard to separation margin, stresses, loading, and coupling dynamic torque) and parametric analysis to determine possible coupling modification (when separation margin, stress level or coupling torque

are not acceptable). The report should also consider how the input data variance will affect the results (sensitivity analysis).

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SPEED OF CONVERGENCE AND ECONOMIC POLICY INSTRUMENTS

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KEYWORDS

Speed of Convergence, Growth Model, Public Policies

ABSTRACT

This article presents an innovative methodology to empirically evaluate the response of the rate of convergence in the neoclassical growth model to changes in the conditional factors. We apply this method to test the sensitivity of the speed of convergence in the EU-15 during the period 1980-2002 to increases in human and public capital.

INTRODUCTION

The relation between private productivity and policy instruments has been a topic of considerable interest in the literature on economic development. A key aspect in the literature on convergence has been the determination of the speed of convergence towards the stationary state. This is determined by its own structural characteristics, among which technology, public policies and the population growth rate are included. Recently, in the debate on convergence, the role played by these conditioning factors has gained prominence – primarily public policy instruments – with the objective of establishing whether part of the observed convergence (if any) can be attributed to these instruments.

In the context of the EU, development and cohesion policies have primarily supported public investment in infrastructures and in education, in addition to support policies for the private sector during the last 20 years. The analyses carried out suggest that these efforts have contributed positively to the process of convergence in productivity in the EU (Salinas *et al.*, 2006). However, recent difficulties encountered in relation to the reduction of disparities in the EU have led to

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) questioning to what extent the speed of convergence could be altered by means of public policies in the European Union. In spite of a clear interest in this matter, few papers have analyzed the sensitivity of the speed of convergence and the majority are theoretical research papers (Turnovsky, 2002, Gokan, 2003, Klump et al., 2008). Unlike these works, in this article a methodological proposal is put forth to estimate the response of the speed of convergence in the EU to changes in economic policy instruments. The analysis proposes two scenarios of convergence: the first one will make it possible to estimate the effect on the speed of convergence arising from changes in the instruments in the EU as a whole; and a second scenario where the effect on the speed of convergence resulting from changes in each one of the countries is considered separately. In this way an attempt will be made to identify not only the potential of various public policies to influence European convergence, but also the role they may play in each country toward achieving convergence in the EU. The proposal develops various scenarios with Matlab that will make it possible to evaluate the sensitivity of the parameter of convergence in the face of variations in the analyzed determining factors, while the other factors remain ceteris paribus.

The article is structured as follows: in the next section, the proposal for empirically evaluating the sensibility of the speed of convergence in the face of changes in the conditioning factors is presented. Section 3 describes the data and presents the findings. Finally, in Section 4, the primary conclusions are presented.

CONDITIONAL CONVERGENCE AND SENSITIVITY ANALYSIS

As of the research carried out by Mankiw *et al.* (1992) and Barro y Sala-i-Martin (1995), the neoclassical growth model is commonly used in order to contrast

conditional convergence. The metodology proposed to examine the response of the rate of convergence consists of the estimation of the convergence equation, recovery of the structural parameters and evaluate the sensibility of the parameter of convergence under specific assumptions about changes in the model. In addition, we simulate those changes - In the estimation of the model we used the routine programming in Matlab available in http://www.spatialeconometrics.com/. The simulations programming in Matlab for this work are available on request- by introducing an extension in the neoclassical growth model. To do so, the fixed effects model provides the basis -. The estimation method is determined by the Matlab programming used to perform the sensitivity analysis. Since GMM approach is suitable to deal with growth models in empirical work, we have also estimated the model with this method and we have reached similar results -, where it is assumed that each explanatory variable has a single coefficient; that is, it has the same effect on the dependent variable, while each individual variable has a different constant which represents the individual effect. Formally, the model to be estimated is the following:

$$\ln\left(\frac{y_{i,t}}{y_{i,t-1}}\right) = \mu + \beta \ln(y_{i,t-1}) + \alpha \ln(x_{i,t}) + \delta \eta_i + u_{i,t}; (1)$$

where y_{it} is the annual GDP per employee of i=1,...,N countries (N=15) and for an annual period of t=1,...,T (T=22 from 1980 until 2002); $x_{i,t}$ is a vector of $k \times 1$ explanatory variables; η_i is the individual effect; and $u_{i,t}$ is a disturbance term. In this case, the concept of conditioned convergence is analyzed by introducing heterogeneity in the model by means of the introduction of fixed effects and/or the effect of other variables, $x_{i,t}$, assuming that the fixed effects η_i are correlated with them.

The estimation of the model (1) is carried out in deviations with respect to the mean using Ordinary Least Squares (OLS), making it possible to consistently estimate the parameters of the model associated with convergence- β and with the explanatory variables since its consistency will not depend on the specification of fixed effects η_i which have been eliminated with the transformation. This estimation is also equivalent to estimating with the OLS model (1) or the model with the variables transformed by orthogonal deviations, a transformation proposed by Arellano (1988) - Given the model $y_{i,t} = \alpha x_{i,t} + \eta_i + u_{i,t}$ he defines the transformation in orthogonal deviations as: $\tilde{y}_{i,t} = \frac{(T-t-1)}{T-t} \left[y_{i,t} - \frac{1}{(T-t-1)} (y_{i,(t+1)} + \dots + y_{i,T}) \right]^{-1}$

The extension of the estimated model (1) takes place through the introduction of changes (simulated increases) in exogenous variables of interest. The simulated increases are based on the minimum of the selected variable and they continue increasing with a fixed value, inc, until reaching a maximum value that, in this case, has been fixed at 100%, since the variables are taken as the percentage of GVA; but both the minimum value as well as the maximum value could be modified with absolute flexibility. The variations generated with Matlab are then placed in rows, until they complete a column, and they continue being placed in the first row of the next column until it has been completed - as has been mentioned above - and the same process continues likewise until a maximum value of 100% is reached. Therefore, the number of columns will depend on the increase inc selected, which in our paper is 5%. Furthermore, the analysis of the variations has been approached in two ways:

a. Evaluating variations of all of the countries at the same time:

$$\Delta(X_{t})_{T\times S} = \begin{bmatrix} \Delta_{1,1} = -\min(X_{t}) & \Delta_{2,1} = \Delta_{1,T} + inc & \dots & \Delta_{S,1} = \Delta_{S-1,T} + inc \\ \Delta_{1,2} = \Delta_{1,1} + inc & \Delta_{2,2} = \Delta_{2,1} + inc & \vdots & \Delta_{S,2} = \Delta_{S,1} + inc \\ \vdots & \vdots & \ddots & \vdots \\ \Delta_{1T} = \Delta_{1,T-1} + inc & \Delta_{2,T} = \Delta_{2,T-1} + inc & \dots & \Delta_{S,T} \approx 100\% \end{bmatrix}; (2)$$

or vectorially:

$$\Delta_{i}(X_{t}) = [\Delta_{1,t}(X_{t}), \Delta_{2,t}(X_{t}), \dots, \Delta_{S,t}(X_{t})]; (3)$$

b. Evaluating variations of a specific country:

$$\Delta^{i}(x_{i,i})_{T \times S} = \begin{bmatrix} \Delta^{i}_{1,1} = -\min(x_{i,i}) & \Delta^{i}_{2,1} = \Delta^{i}_{1,T} + inc & \dots & \Delta^{i}_{S,1} = \Delta^{i}_{S-1,T} + inc \\ \Delta^{i}_{1,2} = \Delta^{i}_{1,1} + inc & \Delta^{i}_{2,2} = \Delta^{i}_{1,1} + inc & \vdots & \Delta^{i}_{S,2} = \Delta^{i}_{S,1} + inc \\ \vdots & \vdots & \ddots & \vdots \\ \Delta^{i}_{1,T} = \Delta_{1,T-1} + inc & \Delta^{i}_{2,T} = \Delta^{i}_{2,T-1} + inc & \dots & \Delta^{i}_{S,T} \approx 100\% \end{bmatrix}; (4)$$

or vectorially as:

$$\Delta_{j}^{i}(x_{i,t}) = [\Delta_{1,t}^{i}(x_{i,t}), \Delta_{2,t}^{i}(x_{i,t}), \dots, \Delta_{S,t}^{i}(x_{i,t})] ; (5)$$

Estimations of the model (1) and the vectors of (3) and (5) with the simulated variables will be used in order to carry out the estimations of the effects of specific explanatory variables that could be used as an instrument of economic policy, while the other variables remain *ceteris paribus*, in order to evaluate the effects on convergence gathered in parameter β .

Generically, the effect of introducing the increase of the exogenous variable for all of the countries can be evaluated with the following model:

$$\ln\left(\frac{y_{i,t}}{y_{i,t-1}}\right) - \hat{\alpha}\ln(x_{i,t}^{l\neq m}) = \mu + \beta\ln(y_{i,t-1}) + \gamma\ln(x_{i,t}^{m} + \Delta_{j}) + \delta\eta_{i} + u_{i,t};$$
(6)

where $\Delta_{j,t}$ is a column vector, corresponding to column *j* which incorporates the gradual increases for t = 1, ..., T for the explanatory variable $x_{i,t}^m$ of each country, to be evaluated of the *k* exogenous variables , being l = 1, ..., k. In this way, j = 1, ..., S estimations of the model (6) are carried out, resulting in different values of the parameter of convergence β .

In particular, the effect of variations on the variable of a specific country can be evaluated, estimating the model:

$$\ln\left(\frac{y_{i,t}}{y_{i,t-1}}\right) - \hat{\alpha}\ln(x_{i,t}^{l\neq m}) = \mu + \beta\ln(y_{i,t-1}) + \gamma\ln(x_{i,t}^{m} + \Delta_{j}^{i}) + \delta\eta_{i} + u_{i,t};$$
(7)

where $\Delta_{j,t}^{i}$ is a column vector, corresponding to column *j* which incorporates the gradual increases for t = 1, ..., T for the explanatory variable $x_{i,t}^{m}$ of country *i*, to be evaluated of the *k* exogenous variables, being l = 1, ..., k. In this way, j = 1, ..., S estimations of model (7) will be carried out for the i = 1, ..., N countries, resulting in different values of the convergence parameter β for each country.

DATA AND RESULTS

The study refers to the EU-15 countries and covers the period 1980-2002. The data used come from World Development Indicators (2005). This database contains information for employment, population, gross value added (GVA) and gross investment expressed in constant terms that are homogenized with purchasing power parity (PPP constant international US\$ in the year 2000). Data on public education expenditure is taken from OECD Education at a Glance and expressed in the same terms than the rest of variables.

Table 1: Variables employed

<i>y</i> _{it}	GVA per worker (PPP international
-	dollars in the year 2000)
S.	Private investment as a percentage of
D _{kit}	GVA
S	Public investment as a percentage of
S_{git}	GVA
S.	Public investment in education as a
$\mathbf{S}_{\mathrm{h}it}$	percentage of GVA
g	Rate of exogenous technical change
	constant and equal to 0.02

n _{it}	Rate of population growth by worker's age
δ	Rate of capital depreciation constant and equal to 0.03

Below the scheme developed in the previous section has been applied to the data on the EU. To do so and in the first place, the equation (1) is estimated by applying the model of fixed effects proposed above - The obtaining of the convergence equation can be consulted in Delgado and Alvarez, (2001) -. The Wald test statistics show that the explanatory variables introduced in the analysis are conjointly significant.

Table 2: Estimation of Convergence Equation with time variable $ln(y_{it-it}/y_{it-it-1})$

Independent variables	Data panel model with fixed effects
$\begin{array}{c} ln(y_{it\text{-}1})\\ lnS_k\text{-}ln(n+g+\delta)\\ lnS_g\text{-}ln(n+g+\delta)\\ lnS_h\text{-}ln(n+g+\delta) \end{array}$	-0.063 (-3.12)** 0.024 (1.67) 0.01 (1.89)* -0.015 (-1.36)
Speed of convergence λ	0.06
Test F Individual effects Hausman Test Wald F Test	$F(14,309)=4.49 \\ \chi^{2}(6)=7.27 \\ F(6,309)=4.9$

The t-ratios shown in parentheses (). * *Significant parameter at 90%, ** at 95%.*

The results of the estimation show a significant, positive speed of convergence that is in line with the most recent papers where it is proven that in recent decades the convergence process in the EU has intensified. The estimations carried out also make it possible to obtain some results as to the influence of the different variables related to public policies developed in European economies: public provision for infrastructures and education. In the first place, a positive and significant influence of public investment on the growth rate of European countries is derived from the analysis carried out. Significant results are not obtained for human capital, although this is a common finding in the literature, given the difficulties that arise when approaching this productive factor.

In order to detect the effect of changes in the economic policy instruments on the sensitivity of the speed of convergence equations, (6) and (7) were estimated. These equations were estimated with Matlab and, in all of the simulations, the values of the previously obtained parameters in the convergence analysis were used. In this study, the analysis focused precisely on the two primary policies developed within the European Union in recent decades: public investment and education expenditure - The programming used will make it possible to carry out this analysis for any of the conditioning convergence factors proposed in the model -.

Figure 1 presents the sensitivity function of the speed of convergence with respect to changes in the rate of public investment. The origin represents the result of the estimation of the speed of convergence with data on the EU-15. The graph shows that for the increase interval of the public investment rate, which is approximately between 0 and 30%, a positive response is obtained for the rate of speed, favoring convergence among member states. Another result of interest is that there is a limit to the capacity of public investment to encourage convergence, changing the track record of the beta convergence if public investment continue to growth. These are important findings since it endorses public policies devoted to increasing public infrastructures in European states but also show that we must take into account other factors that can conditioned their capacity to influence in growth (this is the case of private capital) and therefore high increases in public investment could not achieve the expected results.



Figure 1: Response of β to changes in the rate of public investment

• Figure 2 represents the same analysis, but focusing in the sensitivity of the speed of convergence with respect to the changes in the public investment rate of each European economy separately. The graphs represent the effect on beta of changes in the rate of public investment in each one of the countries under study. In this case, we observed a negative response for the rate of speed for the increase interval in the rate of public investment between 0 and 5% in each country. From this interval, the increases in the rate of investment will not have response in the rate of convergence. The only exception is Greece, which increases the rate of investment greater than 5% achieve a positive effect on the speed of convergence.



Figure 2: Response of β to changes in the rate of public investment by country

• Figure 3 presents the sensitivity function of the speed of convergence with respect to the changes in the rate of public expenditure on education in the European Union. The graph shows that the increase interval of the rate of expenditure on education that influences the speed of convergence is greater than for the public investment (between 0 and 40%). In this case, we also find a limit to the capacity of public expenditure on education to encourage convergence.



Figure 3: Response of β to changes in the rate of expenditure on education

• Figure 4 presents the analysis of sensitivity by country. The results show that the increase in the rate of expenditure on education in each one of the countries studied separately favors the speed of convergence in all cases, with the only exception of Netherland and Luxembourg. Another aspect to

highlight is that the ability to influence is limited to the range of 0 to 20%, being much lower in the cases of Germany, Spain and France.



Figure 4: Response of β to changes in the rate of expenditure on education by country

CONCLUSIONS

The methodology proposed in this paper has made it possible to analyze the sensitivity of the speed of convergence with respect to simulated changes in the economic policy instruments, specifically public and human capital. Our result on the speed of convergence of the EU-15 showed that it depends on the increases of public and human capital accumulation, but that, not surprisingly, there is a limit to their ability to favour convergence.

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Simulation-Based Heuristic Optimization of a Traffic System

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KEYWORDS

Discrete Simulation, Traffic System, Optimization, Heuristics, Simulated Annealing.

ABSTRACT

This paper deals with nonlinear optimization of a stochastic system via simulation and a heuristic algorithm. These tools are used for optimization of the time parameters of the traffic lights of three junctions at Konečného square in Brno, Czech Republic, in order to reach maximum possible throughput. The objective is to minimize average waiting time in the system that might be described as an open queuing network. This is done in two steps: building a simulation model of Konečného square in Java using SSJ (Stochastic Simulation in Java - a Java library for stochastic simulation) and implementing a heuristic algorithm Simulated Annealing that is using the simulation model for optimization. After a brief description of the traffic system, its mathematical and simulation models are introduced. Then the way of getting input data is discussed as well as verification and validation of the simulation model. The results of an optimization based on Simulated Annealing are shown and interpreted in the last part of the paper. Another contribution of building the simulation model is evaluating the effect of implementing the preference given to public transportation.

TRAFFIC SYSTEM

The traffic system at Konečného square in Brno, Czech Republic consists of three complicated junctions of streets Veveří-Kotlářská, Veveří-Nerudova and Úvoz-Žižkova, controlled by traffic lights, shown in figure 1. To simplify the problem we did not consider other neighbouring junctions because they are far enough. Technical documentation was provided by Brněnské komunikace a.s. (BKOM).

Principles of controlling a signalized intersection: Traffic states are described by using phases. During each phase vehicles pass through the junction in directions that are not collisional. A periodical sequence of the phases given by the phase diagram determines how vehicles pass through

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) the junction. Timing of the phases is determined by a signal plan that controls the traffic lights. The longer the phase lasts, the longer queues of vehicles in other collisional directions are formed. The signal plan must satisfy various constraints given by the geometry of the junction, by the obvious requirement to avoid collisions and by various timing constraint resulting from security rules. An intuitive formulation of the problem can be stated as follows:

Find the phases timing in order to maximize the junction throughput while keeping all constraints satisfied. To measure the throughput by a single scalar value, we use the average waiting time spent by a vehicle in the system.



Figure 1. Cartographic Plan of the Konečného Square.

MATHEMATICAL MODEL

As mentioned above, the traffic system can be described as an open queuing network depicted in figure 2. Such systems are obviously stochastic, because some variables are not deterministically fixed. The random k-vector $\boldsymbol{\xi}$ in the objective function $f(\mathbf{x},\boldsymbol{\xi})$ represents all variables whose values cannot be found or computed exactly and are thus characterized by probability distributions. The *n*-vector \mathbf{x} represents the timing plans of all three junctions in the system. Its size is due to different geometries of the junctions equal to n = 11+20+16 = 47 where the three numbers are the numbers of traffic phases in timing plans of the junctions.

If the time intervals between vehicle arrivals and times spent by vehicles in the junctions had exponential distributions, the network could be characterized as an Open Jackson Network and the problem might be solved by standard tools of Queuing Theory. But these distributions are not exponential and therefore as the first approach we substituted them by rather realistic triangular distributions that can easily be changed later. Due to this reason the only feasible method available for evaluation of particular timing plans is simulation.



Figure 2. Queuing Network Representing the Konečného Square, (the inner lines are the trams).

Stochastic programming

To evaluate the objective function describing the performance of the traffic system, a simulation model of the Konečného square was built, since an analytical form of the function f cannot be found due to the randomness and also the complexity of the system. So using the Stochastic Programming terminology we solve the following underlying problem

 $\min_{\mathbf{x}} \{ f(\mathbf{x}, \boldsymbol{\xi}) \mid \mathbf{x} \in C = \{ \mathbf{x} \in U \mid \mathbf{g}(\mathbf{x}) \circ \mathbf{0} \} \},\$

where the vector function $\mathbf{g}: \mathbb{R}^n \to \mathbb{R}^m$ represents all constrains on $\mathbf{x} \in U \subset \mathbb{R}^n$ representing time setting of the phases. *C* is the feasible set, *U* is the domain space of the decision variables \mathbf{x} . There are two categories of the constraints \mathbf{g} . First there are timing constraints represented by lower and upper bounds on all 47 timing periods and also by lower and upper bounds on the duration of the cycles. Another obvious restriction is the stability of the

queueing system. As the effective arrival and service rates depend on **x** in a way that cannot be expressed analytically, this type of feasibility can only be checked by simulation. That's why we define stability by limits on queue lengths L_Q^i in all nodes. These limits are treated differently according to the node type. Exceeding queue length limits in nodes that are entry points into the system represents system instability and it aborts the simulation. That also saves time during the optimization process. Reaching queue length limits in inner nodes represents the temporary saturation of the particular direction. Vehicles are not allowed to enter this queue and are thus forced to stay where they are, but simulation is not aborted. This mechanism also models the obvious limited capacity of road areas intended for waiting vehicles.

To solve the above problem we have to create its deterministic equivalent. We use the so-called Expected Objective (EO) deterministic equivalent where expectation is taken from all times spent by vehicles in the system queues. In particular we define the mean value W_Q^i of waiting times w_{Qi}^j in the queue of the *i*-th node,

 $W_Q^i = \frac{1}{n_i} \sum_{j=1}^{n_i} W_{Qj}^i$, where n_i is the total number of cars that

went through the node *i* during the experiment run. These mean waiting times are then weighted by the total numbers of cars in the nodes. This is the objective function formula:

$$f(\mathbf{\kappa}(\mathbf{x}),\boldsymbol{\xi}) = a + qs + \frac{\sum_{i=1}^{N} n_i(\mathbf{\kappa}(\mathbf{x}),\boldsymbol{\xi}) W_{\mathcal{Q}}^i(\mathbf{\kappa}(\mathbf{x}),\boldsymbol{\xi})}{\sum_{i=1}^{N} n_i(\mathbf{\kappa}(\mathbf{x}),\boldsymbol{\xi})}$$

where the function κ represents the configuration parameters of the simulation model and N is the number of nodes (queues) of the model.

The objective function f thus represents the weighted average of the average waiting times in the queues of the system, which is further penalized for breaking constraints (i.e. if $\mathbf{x} \in U - C$). The weights are defined as relative frequencies of vehicles detected in the queues. s is the penalization for breaking one constraint, q is the number of broken constraints and a is the penalization for aborted simulation that occurs if maximal queues lengths in entry nodes are exceeded for a generated solution \mathbf{x} . A big value of a is used to represent infeasibility of the particular solution.

SIMULATION MODEL

The simulation model was written in Java with the use of the SSJ (Stochastic Simulation in Java) tool. SSJ is a Java library for stochastic simulation, developed under the direction of Pierre L'Écuyer, in the Département d'Informatique et de Recherche Opérationnelle (DIRO), at the Université de Montréal. It provides facilities for generating uniform and nonuniform random numbers, computing different measures related to probability distributions, performing goodness-of-fit tests, applying quasi-Monte Carlo methods, collecting (elementary) statistics, and programming discrete-event simulations with both events and processes paradigm. For more detailed description of the tool see for example (L'Ecuyer and Buist 2005) or visit the homepage of the tool at http://www.iro.umontreal.ca/~simardr/ssj/indexe.html.

Abstract model

The abstraction is based on usual continuous time, discrete behaviour paradigm. The state of the system is changed when an event occurs, for example a vehicle arrival. This change takes no time and the state does not change between two adjacent events. As mentioned above, random variables occur in this system and thus the system is also stochastic. Vehicles movement is modelled by Java objects of the type *Event*.



After generating an arrival interval with mean $1/\lambda_i$, a new car is generated at system input and passed into the particular queue. If there is a green light on and the queue length is 1, the car is taken out from the queue, the waiting time is saved and queue length is updated. The car is then passed to the server, representing queue emptying, where it waits an average time $1/\mu_i$. Then it is removed and sent to the next node or out of the system. In case that the car reaches a branching node, the probability of selecting the next direction is given by statistical measurements from cartograms provided by BKOM. Parameters of triangular distributions that define the rates λ_i and μ_i for each node are based on statistical measurements performed on the real system by Zdislav Beranek.

Control of the traffic lights is modelled by SSJ objects of the type *SimProcess*. The control can run in two different modes with or without preference given to the public transport. In case of public transport preference mode there is a special phase turned on if a public transport vehicle is coming. The phase allows a requesting vehicle to pass through the junction without a too long waiting.

The more important model simplifications are these:

- Simplification of some traffic priority rules.
- No vehicles with higher priority (e.g. ambulance) are considered in the model.
- No accidental breaking of traffic rules.

- Missing traffic lights states "ready" orange because they overlap with green and red phases. Orange before green is considered as red, orange before red is considered as green.
- Triangular distribution for generating time intervals between vehicles arrivals.
- Triangular distribution for generating time intervals that simulate passing of vehicles through the junctions.

Verification and validation of the model

The verification of the simulation model was done by comparing results with visualization software VISSIM provided by BKOM, which were obtained in two steps:



Figure 4. Measured Segments of Konečného Square

At the segments depicted in the figure 4, the maximal queues lengths and the average waiting times in these queues were measured. These waiting times from VISSIM were then compared with the ones obtained from the simulation model.

The simulation time was 72000s (20h), statistics collection started after the first 300s warming period. The used mode was without public transport preference. To compare the results see the tables 1, 2 and 3.

A significant difference occurred at segment 17, data of streets Úvoz VC, VD, VE in the table 3, are missing, because of VISSIM incomplete implementation.

With respect to effort of engineers of BKOM and that the VISSIM is working with real time, there is no such comparison for a mode implementing public transport preference. In this case we accepted an opinion of a traffic specialist from BKOM, who considers the model implementation to be correct.

To validate the model with public transport preference a new statistical measurement of the junctions would have to be performed for comparing the results. Due to high cost this was not acceptable.

Table 1. Average Waiting Times at Junction Veveří-Kotlářská

Segment	Street	Simulation model [s]	VISSIM [s]
23	Veveří VA	2.8	5.4
18	Kotlářská VB	30.6	45.2
16	Veveří VC	28.8	34.4
25	Úvoz VD	21.6	18.2

 Table 2. Average Waiting Times at Junction Veveří-Nerudova

Segment	Street	Simulation model [s]	VISSIM [s]
23	Veveří VA	28.8	30.3
24	Nerudova VB	40.0	54.7
17	Veveří VC	38.1	6.9
21	Úvoz VD	21.6	18.2

Table 3. Average Waiting Times at Junction Úvoz-Žižkova

Segment	Street	Simulation model [s]	VISSIM [s]
26	Nerudova VA	10.4	9.5
19	Kotlářská VB	8.8	10.5
20	Úvoz VC	39.4	
	Úvoz VD	2.4	
	Úvoz VE	4.0	

OPTIMIZATION

As we have just numerical approximation of the objective function *f* given by the simulation model (together with checking the feasibility), we are limited in selection of the optimization algorithm. First we believe that all algorithms based on differentiability (like for example gradient based methods) are not appropriate because of two reasons. First numerical computation of gradients needs extra function evaluations that means additional simulation runs. Second, close to optima norms of gradients tend to become small, possibly much smaller than errors involved in approximation of the objective function by simulation. So we are limited to use either exact or heuristic algorithms based on function evaluation only. From these algorithms we have chosen the heuristic optimization algorithm Simulated Annealing (SA).

Simulated Annealing Algorithm

1. set(
$$c$$
, $x_{current}$);
2. $x_{current} \rightarrow x_{best}$;
3. do{
4. update(c);
5. do{
6. get(x_{new});
7. if($f(x_{new}) < f(x_{best})$){
8. $x_{new} \rightarrow x_{best}$;
9. }
10. if($f(x_{new}) < f(x_{new})$)

10. if $(f(x_{new}) \le f(x_{current}))$ {

11. $x_{new} \rightarrow x_{current}$; 12. } 13. else if (random(0,1) $\leq \exp\left(-\frac{f(x_{new}) - f(x_{current})}{c}\right)$) { 14. $x_{new} \rightarrow x_{current}$; 15. } 16. } while(we are not enough close to equilibrium) 17. } while(system is not frozen)

Decreasing control parameter *c* is referred to as the annealing temperature. Frozen system represents a found heuristic solution $(c \approx 0)$. The so-called Metropolis criterion (line 13) allows the algorithm to get out of a local minimum. Thermal equilibrium, for a given *c*, is determined by the probability of being in a configuration \mathbf{x}_{i+1} that is characterised by the so-called energetic state *E*. The probability is given by Boltzmann distribution:

$$\mathbb{P}\left[E = f\left(\mathbf{x}_{i+1}\right) - f\left(\mathbf{x}_{i}\right)\right] = \exp\left(-\frac{f\left(\mathbf{x}_{i+1}\right) - f\left(\mathbf{x}_{i}\right)}{c}\right)$$

Heuristic algorithms give good solutions, they cannot guarantee reaching global optimum. However a proof of convergence of SA exists, see (Laarhoven 1989). The performance of the implemented algorithm depends on its setting, generally called cooling schedule.

Cooling schedule

- Setting of the initial value of *c* is done in such a way that virtually all values of **x** could be accepted. There is an acceptance ratio χ_a defined as the number of accepted **x** to all tested **x**. If χ_a < χ₀, the pre-initial temperature *c̃* is raised to *c̃*_{i+1} = 2*c̃*_i. Final temperature *c̃* equals to *c* initial. For optimization we used χ₀ = 0.8, *c̃*₀ = 50.
- The final value of *c* is used to stop SA if no better solution was found for a longer time. In a similar way as above there is a rejection ratio χ_r defined as the number of rejected **x** to all tested **x**. If $\chi_r \ge \chi_f$, the algorithm stops. We used $\chi_f = 0.7$.
- To approximate the equilibrium for a given c_k a minimal number of perturbations (x_i → x_{i+1}) must be accepted. But for c_k → 0 this number goes to infinity. Therefore the number must be also limited by a maximal value. For optimization we used min = 5 and max = 14.
- It is recommended to decrease the control parameter *c* as slowly as possible. In this case it is exponential $c_{k+1} = 0.9c_k$.

Two configurations \mathbf{x}_i , \mathbf{x}_j are statistically compared via Mann-Whitney test. A requested number of observations \hat{f} of the objective function f for each of the configurations is provided via simulation and then these sets are tested. For optimization the confidence level was 0.05 and the number of observations was 7.

Optimization results

The system is optimized only in the mode without the public transport preference, because otherwise the system is not stable (see figures 5, 6) for original configuration designed by BKOM. Penalization constants in the objective function formula were s=100 and a=400. Based on the testing of stability and variability, the time horizon 172,800s of a simulation and statistics collection restart in 600s were determined. The duration of the optimization was about 7 h (real time).

Graphs in figures 5 an 6 display objective function values for various time horizon lengths.



maxTime 360000s dt 3600s preference true timeRestartStat 600s singlePenalty 100 abortPenalty 400



numOfSim 50 timeHorizon 54000s preference true timeRestartStat 600s singlePenalty 100 abortPenalty 400



Figure 5 is for public transport preference, in the figure 6 there are results for simulations without public transport preference. The configurations \mathbf{x} are the same, designed by BKOM. The vertical axis is the objective function value, the horizontal axis is the simulation duration in seconds and the number of the simulation experiments respectively. The figure 5 shows that the mode with public transport preference is unstable because there is not enough time for other than public transport vehicles. This result corresponds with reality. The junctions are currently set to no preference to public transport mode.

Tables 4, 5, 6 contain the optimization results for the mode without public transport preference. Only the lengths of main phases (written in black frames in tables 4, 5, 6) were optimized. Other phases arrange a safe switch between the main phases. They are determined mainly by the constraints, so there is no sense in changing them. The tables 4, 5, 6 show current implementation of signal plans for which the average value of the objective function equals to 19.392 and the optimized signal plan configuration for which the average value of the objective function is 15.595.



maxTime 360000s dt 3600s preference false timeRestartStat 600s singlePenalty 100 abortPenalty 400



numOfSim 50 timeHorizon 172800s preference false timeRestartStat 600s singlePenalty 100 abortPenalty 400

Figure 6. Stability and Variability of Simulation in Mode without Public Transport Preference.

Table 4. Optimization Results

	Traffic	phases timing at Veveří-Kotlá	ářská	
	going directions	stopped directions	current	otpimized
	VB, VD, PA, PC	VA, VC, TA, TC, PB, PD	8	18
			7	7
			1	1
			5	5
			1	1
ases	VA, VC, TA, TC, PB, PD	VB, VD, PA, PC	37	37
hd			3	3
	VA, VC, TA, TC	VB, VD, PA, PB, PC, PD	9	4
			5	5
			1	1
	VB, VD, PA, PC	VA, VC, TA, TC, PB, PD	23	19

Table 5. Optimization Results

	Troffic nh		davra	
	Tramic pro	ases timing at veveri-neru	dova	
	going directions	stopped directions	current	optimized
	VD, KD, SA, TBS,	VA, VB, VC, SC, TA,	2	3
	TBP, TCL	TBL, TCS, TCP, PA, PB,		
		PD		
			2	2
			2	2
			3	3
			1	1
	VB. SC. TBL. TBS.	VA. VC. VD. KD. SA. TA.	7	10
	TBP, TCL, TCP, PA	TCS, PB, PD	-	_
	, , ,	, ,	8	8
			1	1
			5	5
ŝ			1	1
ase			1	1
he			8	8
~			5	5
			5	3
	VA, VC, TA, TBS,	VB, VD, KD, SA, SC,	15	20
	IBP, ICL, ICO,	TBL, TCP, PA		
	PB, PD		-	4
			1	1
			4	4
			1	1
			4	4
	VD, KD, SA, TBS,	VA, VB, VC, SC, TA,	29	21
	TBP, TCL	TBL, TCS, TCP, PA, PB,		
		PD		

Table 6. Optimization Results

	Traffic pl	hases timing at Uvoz-Zižk	ova	
	going directions	stopped directions	current	optimized
	VB, PA, VD, VE	VA, VC, SC, PB, PE, PD	18	21
			5	5
			3	3
			2	2
			1	1
			2	2
Ś	VA, PB, PE, PD	VB. VC, SC, PA, VD, VE	7	1
se			10	10
ha	VA, PB, PE, VD, VE,	VB, VC, SC, PA, PD	6	2
<u>u</u>			6	6
	VA, VC, PE, VD, VE	VB, SC, PA, PB, PD	27	37
			2	2
			5	5
			1	1
	VB, SC, PA, VD, VE	VA, VC, PB, PE, PD	2	3
	VB, PA, VD, VE	VA, VC, SC, PB, PE, PD	3	0

Most of directions from tables 4, 5 and 6 can be found in the figure 1. Directions starting with the letter P mark

traffic lights for pedestrian crossings, Directions starting with S or K mark additional traffic directions which help to decrease the queues. The third character in TBP, TAL, TCS, etc. clarifies tram directions: right (P), left (L), and middle (S) respectively.

Tables 7, 8 and 9 compare the average queue length, the maximal number of vehicles in the queue and the average waiting time in all queues.

	Current configuration			Current configuration Optimized configuration		guration
street	\overline{L}_{ϱ}	$\max L_{\!\mathcal{Q}}$	$ar{W}_{\!\mathcal{Q}}\left[\mathbf{s} ight]$	\overline{L}_{Q}	$\max L_{\varrho}$	$ar{W}_{\!\mathcal{Q}}\left[s ight]$
Veveří VA	0.47	6.00	2.81	0.77	8.00	4.56
Kotlářská VB	6.58	33.00	32.09	4.89	19.00	23.81
Veveří VC	3.79	13.00	29.01	4.02	13.00	30.69
Úvoz VD	2.86	18.00	21.14	3.71	20.00	27.31
Veveří TA	0.02	2.00	3.59	0.06	2.00	8.71
Veveří TC	0.08	1.00	11.95	0.10	1.00	15.19

Table 6. Juliculoli veveli-ineruuov	Table	8.	Junction	Veveří-Nerudova
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	Current configuration			Optimized configuration		
street	\overline{L}_Q	$\max L_{\mathcal{Q}}$	$\overline{W}_{\!\mathcal{Q}}\left[\mathbf{S} ight]$	\overline{L}_{Q}	$\max L_{\mathcal{Q}}$	${{ar W}_{\!\mathcal Q}}\left[{{\mathbf{s}}} ight]$
Veveří VA	5.89	23.00	27.62	4.50	16.00	21.09
Nerudova VB	1.96	6.00	40.03	1.80	6.00	36.98
Veveří VC	5.24	25.00	38.36	2.41	15.00	17.83
Úvoz VD	0.66	8.00	4.59	2.87	20.00	20.01
Veveří TA	0.07	1.00	21.76	0.06	1.00	18.96
Veveří TB	0.12	1.00	36.70	0.11	1.00	33.84
Veveří TC	0.09	1.00	13.38	0.07	1.00	10.33

Table 9. Junction Úvoz-Žižkova

	Current configuration			Optimized configuration		
street	\overline{L}_Q	$\max L_{\mathcal{Q}}$	$\overline{W}_{\mathcal{Q}} \left[\mathbf{S} ight]$	\overline{L}_Q	$\max L_{\mathcal{Q}}$	${\it W}_{\!\scriptscriptstyle Q}$ [s]
Nerudova VA	0.93	9.00	10.50	0.96	9.00	10.93
Kotlářská VB	1.22	13.00	8.94	1.02	11.00	7.41
Úvoz VC	11.35	46.00	39.17	6.37	21.00	21.99
Úvoz VD	0.70	9.00	2.43	0.37	7.00	1.27
Úvoz VE	0.82	9.00	3.99	0.44	7.00	2.12

We can see that most of the observed values decreased in the optimized configuration. Nevertheless the traffic specialists from BKOM have to check the feasibility of the proposed optimized configuration before its possible implementation.

SUMMARY

A traffic system can be very complex and random. The only feasible way of obtaining quantitative information about modifications of such a system is simulation. The simulation model presented in this paper was built in Java with use of the SSJ simulation tool. The user of this simulation model may set a lot of data through a GUI interface and therefore it is possible to compare various settings in a user-friendly way.

It is also an example of the application of simulation methods in operation research. Simulation was used for evaluation of the objective function (weighted average of the average waiting times in the queues of the system) because analytical methods cannot be applied due to the complex and random nature of the system. The objective function was optimized by Simulated Annealing. The optimization of traffic lights configuration was performed and results are shown at the end of the paper. A considerable improvement over the current timing plan was found.

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Model Development and Optimization Base on Generalized Steady-State Electrochemical Equations for a PEM Fuel Cell

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KEYWORDS

PEM fuel cell, Generalized model, Steady-State model, Hybrid Optimization, Genetic algorithm.

ABSTRACT

The development of a generalized steady-state electrochemical model of a polymer electrolyte fuel cell or proton exchange membrane fuel cell (PEMFC) system is presented by R.F Mann et al. to predict the output voltage of a single Ballard Mark V cell as a function of the major variables like current density, pressure of the reactant gases and working temperature more efficiently (Mann et al. 2000). But this model cannot explain the behavior of the voltage at high current densities as well as the other ranges. In this research a new term that account for mass transfer losses is added to compensate the precision of the model particularity at high current densities. Using this model, the power density of a Ballard Mark V fuel cell system that consists of 35 cells is optimized by a hybrid optimization algorithm base on genetic algorithm and a gradient base algorithm that shows very good performance to reach the exact optimum point.

INTRODUCTION

The proton exchange membrane fuel cells (PEMFC) are suitable for portable, mobile and residential applications, due to their inherent advantages, such as high-power density, simple and safe construction and quick startup even at low operating temperatures. Rapid development recently has brought the PEMFC significantly closer to commercial reality.

Although prototypes of fuel cell vehicles and residential fuel cell systems have already been introduced, it remains to reduce the cost and enhance their efficiencies. To improve the system performance, design optimization, analysis and control of fuel cell systems are important. Mathematical models and simulation are needed as tools for design optimization of fuel cells, stacks, and fuel cell power systems. (EG&G Technical Services, Inc. 2004)

Different mathematical models have been devised to simulate the behavior of a PEM-FC. Some are based on curve-fitting experiments or semi-empirical models that

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) combine experimental data with parametric equations adjusted by comparison with cells physical variables like pressure and temperature (Cirrincione et al. 2005). An electrochemical-based fuel cell model is presented by R. F. Mann et al. that leads to a generalized scheme for modeling the PEM fuel cells. (Mann et al. 2000) Also a dynamic electrochemical-based fuel cell model is proposed and developed by J. M. Corrêa et al. that account for concentration overvoltage too. (Corrêa et al. 2004)

Here a generalized steady-state fuel cell model is proposed. The power output of a PEM fuel cell system is then optimized base on this model. The operating variables of the cell are current density and working temperature.

The multi-variable optimization task is then done using a hybrid optimization method base on Genetic Algorithm.

BASIC STRUCTURE

Unit cells form the core of a fuel cell. These devices convert the chemical energy contained in a fuel electrochemically into electrical energy. The basic physical structure, or building block, of a fuel cell consists of an electrolyte layer in contact with an anode and a cathode on either side. A schematic representation of a unit cell with the reactant/product gases and the ion conduction flow directions through the cell is shown in Figure 1. (EG&G Technical Services, Inc. 2004)



Figure 1: Schematic of an Individual Fuel Cell

In a typical fuel cell, fuel is fed continuously to the anode (negative electrode) and an oxidant (often oxygen from air) is fed continuously to the cathode (positive electrode). The electrochemical reactions take place at the electrodes to produce an electric current through the electrolyte, while driving a complementary electric current that performs work on the load. Although a fuel cell is similar to a typical battery in many ways, it differs in several respects. The battery is an energy storage device in which all the energy available is stored within the battery itself. The battery will cease to produce electrical energy when the chemical reactants are consumed (i.e., discharged). A fuel cell, on the other hand, is an energy conversion device to which fuel and oxidant are supplied continuously. In principle, the fuel cell produces power for as long as fuel is supplied. (EG&G Technical Services, Inc. 2004)

In a PEMFC, on a side of the cell, referred as the anode, the fuel is supplied under certain pressure. The fuel for this model is the pure gas H_2 , although other compositions of gases can be used. In these cases, the hydrogen concentration should be determined in the mixture. The fuel spreads through the electrode until it reaches the catalytic layer of the anode where it reacts to form protons and electrons:

$$H_2 \longrightarrow 2H^+ + 2e^-$$
 (1)

The protons are transferred through the electrolyte (solid membrane) to the catalytic layer of the cathode. On the other side of the cell, the oxidizer flows through the channels of the plate and it spreads through the electrode until it reaches the catalytic layer of the cathode. The oxidizer used in this model is oxygen or O_2 . The oxygen is consumed with the protons and electrons and the product, liquid water, is produced with residual heat on the surface of the catalytic particles. The electrochemical reaction that happens in the cathode is:

$$2H^+ + 2e^- + \frac{1}{2}O_2 \longrightarrow H_2O + Heat$$
 (2)

Then, the full physical-chemical FC reaction is (Corrêa et al. 2004):

$$H_{2} + \frac{1}{2}O_{2} \longrightarrow H_{2}O + Heat +$$
ElectricalEnergy
(3)

MODEL DEVELOPMENT

The actual cell potential is decreased from its ideal potential because of several types of irreversible losses. These losses are often referred to as polarization, overpotential or overvoltage, though only the ohmic losses actually behave as a resistance. (EG&G Technical Services, Inc. 2004) The output voltage of a single cell can be defined as the result of the following expression (Mann et al. 2000; Corrêa et al. 2004):

$$V_{cell} = E_{Nernst} + V_{act} + V_{ohm} + V_{con}$$
(4)

Where: E_{Nernst} is the thermodynamic potential of the cell and it represents its reversible voltage; V_{act} is the voltage drop due to the activation of the anode and cathode (also known as activation overpotential), a measure of the voltage drop associated with the electrodes; V_{ohm} is the ohmic voltage drop (also known as ohmic overpotential), a measure of the ohmic voltage drop resulting from the resistances of the conduction of protons through the solid electrolyte and the electrons through its path; and V_{con} represents the voltage drop resulting from the reduction in concentration of the reactants gases or, alternatively, from the transport of mass of oxygen and hydrogen.

In the V-I diagram, especially for low-temperature fuel cells like PEM fuel cells, the effects of these three loss categories are often easy to distinguish, as illustrated in Figure 1(EG&G Technical Services, Inc. 2004):



Figure 2: Actual Fuel Cell Voltage illustration.

The total voltage output of the fuel cell unit with 35 cells connected in series is (Frangopoulos and Nakos 2006):

$$V_{stack} = n_{cell} \times V_{cell} \tag{5}$$

Where n_{cell} is the number of single cells in the PEM fuel cell stack. The instantaneous electrical power supplied by the cell to the load can be determined by (Frangopoulos and Nakos 2006):

$$P_{cell} = JAV_{cell} \tag{6}$$

Where V_{cell} is the cell output voltage for each operating condition and P_{cell} is the output power, in Watts. J is the current density in (A/cm²) and A is the cell active area (cm²). The fuel cell efficiency is given by (Frangopoulos and Nakos 2006):

$$\eta_{cell} = \mu_f \frac{V_{cell}}{1.48} \tag{7}$$

Where μ_f is the fuel utilization coefficient, generally in the range of 95% and 1.48 represents the maximum voltage that can be obtained using the higher heating value (HHV) for the hydrogen enthalpy (for lower heating values or LHV this number is 1.25). Fuel utilization is assumed to be constant, which is valid where the fuel cell has a hydrogen flow rate control. In this case, the hydrogen is supplied according to the load current. (Corrêa et al. 2004) The hydrogen molar consumption rate for the whole fuel cell unit according to the load current is calculated by (EG&G Technical Services, Inc. 2004; Frangopoulos and Nakos 2006):

$$N_{H_2}^{req} = \mu_f \frac{JA}{2F} \times n_{cell} \tag{8}$$

$$m_{H_2}^{req} = \mu_f \frac{JA}{2F} \times n_{cell} \times M_{H_2}$$
(9)

Where F is the Faraday's constant (96,487 coulombs (C)), N_{H2}^{req} is the hydrogen molar consumption rate (molH₂/min), m_{H2}^{req} is the hydrogen mass consumption rate (kgH₂/min) and M_{H2} is the molar mass of hydrogen molecule (gr/molH₂).

Cell reversible voltage

The reversible voltage of the cell (E_{Nernst}) is the potential of the cell obtained in an open circuit thermodynamic balance (without load). In this model, E_{Nernst} is calculated starting from a modified version of the equation of Nernst. This is given by (Larminie and Dicks 2003):

$$E_{Nernst} = \frac{\Delta G}{2F} + \frac{\Delta S}{2F} (T - T_{ref}) + \frac{RT}{2F} \left[\ln(p_{H_2}) + \frac{1}{2} \ln(p_{O_2}) \right]$$
(10)

Where ΔG is the change in Gibbs free energy at standard temperature and pressure (J/ mol), ΔS is the change in entropy at standard temperature and pressure (J/ mol), R is the Molar or universal gas constant (8.314 JK⁻¹mol⁻¹) and p_{H2} and p_{H2} are the Partial pressure of hydrogen and oxygen respectively (atm).

Activation Voltage Drop

Activation losses stem from the activation energy of the electrochemical reactions at the electrodes. These losses depend on the reactions at hand, the electrocatalyst material and microstructure, reactant activities (and hence utilization), and weakly on current density. As shown in (Mann et al. 2000), the anode overvoltage can be represented by:

$$V_{act,a} = -\frac{\Delta G}{2F} + \frac{RT}{2F} \ln(4FAk_a^0 C_{H_2})$$

$$-\frac{RT}{2F} \ln(i)$$
(11)

Where ΔG is the change in Gibbs free energy at standard temperature and pressure (J/ mol), ΔS is the change in entropy at standard temperature and pressure (J/ mol), R is the Molar or universal gas constant (8.314 JK⁻¹mol⁻¹), k_a^0 is the intrinsic rate constants for the anode (cm/s) and C_{H2} is the concentration of hydrogen respectively (molH₂/ cm³).

And the cathode overvoltage can be given by:

$$V_{act,c} = \frac{RT}{\alpha_c Fn} \ln(nFAk_c^0 \exp\left(-\frac{\Delta G}{RT}\right) \times (C_{O_2})^{(1-\alpha_c)} (C_{H_2})^{(1-\alpha_c)} (C_{H_2O})^{(\alpha_c)} - \ln(i)$$
(12)

Where α_c chemical activity parameter for the cathode,

 k_a^0 is the intrinsic rate constants for the anode (cm/s) and C_{H2}, C_{O2}, C_{H2O} is the concentration of hydrogen, oxygen, product water respectively (molH₂/cm³).

If there is a need for a single expression to represent the activation overvoltage, the total expression to represent the activation overpotential, including anode and cathode, can be calculated by (Mann et al. 2000):

$$V_{act} = \xi_1 + \xi_2 T + \xi_3 T \ln(C_{O_2}) +$$

$$\xi_4 T \ln(JA)$$
(13)

Where the ξ 's represent parametric coefficients for each cell model, whose values are defined based on theoretical equations with kinetic, thermodynamic and electrochemical foundations (Mann et al. 2000).

The concentration of hydrogen and oxygen in the catalytic interface of the anode and the cathode respectively are determined by Henry's law and are given by (Corrêa et al. 2004; Frangopoulos and Nakos 2006):

$$C_{H_2} = \frac{P_{H_2}}{1.09 \times 10^6 \times e^{\frac{77}{T}}}$$
(14)

$$C_{o_2} = \frac{P_{o_2}}{5.08 \times 10^6 \times e^{\frac{-498}{T}}}$$
(15)

Which are in (mol/cm^3) .

Ohmic Voltage Drop

The ohmic voltage drop results from the resistance to the electrons transfer through the collecting plates and carbon electrodes, and the resistance to the protons transfer through the solid membrane. In this model, a general expression for resistance is defined to include all the important parameters of the membrane. The equivalent resistance of the membrane is calculated by (Mann et al. 2000; Corrêa et al. 2004):

$$V_{ohm} = JA \left(R_{prot} + R_{elec} \right) = JA R_{int\,ernal} \tag{16}$$

The equivalent resistance of the membrane is calculated by:

$$R_{prot} = \frac{r_m l}{A} \tag{17}$$

Where r_m is the membrane specific resistivity for the flow of hydrated protons (ohm.cm), approximated by the following empirical expression for NafionTM 117 membrane (Mann et al. 2000):

$$r_{m} = \frac{181.6 \left[1 + 0.03 J + 0.062 J^{2.5} \left(\frac{T}{303}\right)^{2}\right]}{\left[\psi - 0.634 - 3J\right] \times e^{\left(\frac{4.18 \left(\frac{T-303}{T}\right)}{T}\right)}}$$
(18)

Where T is the operating temperature of the cell (K) and the parameter ψ is an adjustable parameter with a possible maximum value of 23.

Concentration Voltage Drop

The mass transport affects the concentrations of hydrogen and oxygen. This, by its turn, causes a decrease of the partial pressures of these gases. Reduction in the pressures of oxygen and hydrogen depend on the electrical current and on the physical characteristics of the system. To determine an equation for this voltage drop, it is defined a maximum current density, J_{max} , under which the fuel is being used at the same rate of the maximum supply speed. The current density cannot surpass this limit because the fuel cannot be supplied at a larger rate.

Thus, the voltage drop due to the mass transport can be determined by (Corrêa et al. 2004; Cirrincione et al. 2005):

$$V_{con} = B \ln \left(1 - \frac{J}{J_{\text{max}}} \right) \tag{19}$$

Where B is a constant that depends on the fuel cell and its operating state (V).

EVALUATION AND VALIDATION OF THE MODEL

For implementation of above equation in MATLAB[®] and validation of the model, one single cell, model Ballard Mark V, was simulated, which was fed with gases H₂ and O₂, using the membrane NafionTM 117. The parameters used for this simulation are presented in Table 1(Corrêa et al. 2004):

Table 1: Ballard Mark V single cell parameters

Parameter	Value
А	50.6 cm^2
1	178 μm
p _{H2}	1 atm
p _{O2}	1 atm
В	0.016 V
R _{elec}	0.0003 ohm
ξ1	-0.948
٤	0.00286+0.0002.lnA+(4.3x10-
52	5).lncH2
ξ3	7.6x10-5
ξ4	-1.93x10-4
Ψ	23
J _{max}	1500 mA/cm^2

Figure 3 illustrates the polarization curve predicting by this model versus the experimental data by R. F. Mann et al. (Mann et al. 2000) and the model proposed by J. M. Corrêa et al. (Corrêa et al. 2004) as a reference model to validate the efficiency of the proposed model.



Figure 3: Ballard Mark V polarization curve

Figure 4 and 5 illustrate the efficiency and power density of a single cell base on the proposed model respectively.



Figure 4: Ballard Mark V single cell efficiency



Figure 5: Ballard Mark V Power Density

HYBRID OPTIMIZATION METHOD

A hybrid optimization method is a gradient base optimization method together with genetic algorithm, which is a fast precise optimization scheme. Figure 6 shows the system optimization architecture:



Figure 6: The system optimization architecture

Genetic algorithm is a derivative free and population base algorithm that can near the global optimum point without trapping in other local optimum points. However there is no guarantee to reach the exact global optimum point because it is not gradient base and it is base on some random search. Using this algorithm together with a gradient base optimization method is a very good scheme that shows great performance. Also because of using a gradient base optimization method together with Genetic Algorithm, reaching the exact optimum point is promised.

SYSTEM OPTIMIZATION AND RESULTS

The optimization of the proposed model is done by using a hybrid optimization algorithm. Here the current density and operating temperature are the main system variables where the hydrogen consumption rate for the fuel cell unit is calculated by the equations (8), (9).

The proposed bounds for current density and operating temperature are [0.11 1.31] (A/cm²), [60 90] (°C) respectively.

Using this method for optimizing the power output of the PEM fuel cell unit gives:

 $J^* = 1309.132 \text{ mA/cm}^2$, $T^* = 362.752 \text{ K}$

This leads to the optimum power output of the stack as follows:

 $P = V \times I => P^* = 1.4237e+3 W$

Figure (7) also agrees with the optimization result:



Figure 7: Ballard Mark V Stack Power Output

Figure (8), (9) illustrate a single cell voltage and efficiency in the proposed operating temperature range respectively:



Figure 8: Ballard Mark V single cell Output Voltage



Figure 9: Ballard Mark V single cell Efficiency

From the presented Figures, it can be seen that the cell voltage and efficiency present higher values for low current densities and power densities. On the other hand, for higher values of power, the efficiency and the voltage present smaller values.

CONCLUSIONS

The results of the optimization of a PEM fuel cell stack shows that, besides the reversible cell voltage is higher at low temperature, but higher output power of the stack can be achieved at higher temperature due to higher current and decrease in voltage losses. So for designing a more efficient PEM fuel cell stack, the appropriate balance of plant (BoP) should be designed to compensate the operating temperature and current density to the optimum ones.

It is also important that the system cannot work with a very high voltage or very high current because of some technical issues like decreasing the useful life of the cell. The designer of the control system should decide the appropriate voltage and current in each case with respect to the demand of the plant or grid so that it does not cause a minor or major damage to the cell. A tradeoff between power output and system efficiency must be taken into account too.

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Phenomenal Trust Model

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KEYWORDS

Trust, trust modelling, impersonal trust.

ABSTRACT

The paper deals with the phenomenal trust modelling. Required terms as trust, trust types, trust values and representation are mentioned. Fundamental description of phenomenal trust formation is presented as a form of impersonal trust which is complementary to interpersonal trust. Phenomenon is defined by the set of its possible exclusive values. The model describes the trust of a subject to particular value of a phenomenon. Proposed formula for phenomenal trust formation covers the factors as product reputation, number of recommendations of product, initial trust value of products and trusting disposition of the subject. The behaviour of trust evolution depending on particular factors is studied.

INTRODUCTION

Trust is a unique phenomenon and plays an important role in the relationships among subjects in the communities. In the internet age, the trust among the machines, servers, and network nodes gains more and more on importance. Widening of e-service (Liu et al. 2008), e-commerce (Wang and Zhang. 2008), ebanking, etc., arises the question of human machine trust. Further, trust plays an important role in peer-topeer networks (Wu et al. 2008), ad hoc networks, grid computing, semantic web (Wang and Zhang 2008), and multi agent systems, where humans and/or machines have to collaborate.

What is it trust and how it can be described? The acceptance of trust is wide and various explanations are offered (Fetzer 1988); from honesty, truthfulness, confident expectation or hope, something managed for the benefit of another, confidence in ability or intention to pay for goods or services in the future, till business credit.

The universal trust definition does not exist. Bulk of definitions comes out from Gambetta's definition (Gambetta 2000). We will understand trust as a given credit, hope, confidence in ability or intention of some subject to perform to benefit of other subject at some future time. Trust is created not only among the subjects (persons, nodes), but the subject can be perceived as a phenomenon, i.e. another type of trust – impersonal trust (Alfares and Hailes 2000; Alfares 2005) complementary to interpersonal trust; trust is formed towards a phenomenon, e. g. to certain product from a set of products of some kind.

Interpersonal trust models used for decision on selection of partners can be formed in several ways. The random selection can be the first choice, e.g. (Fort 2003). Further, probability can be applied (Yu et al. 2001), (Winsborough and Li 2002), (Yu and Winslett 2003) and (Rettinger et al. 2007). The game theoretic approach to modeling trust based decisions is proposed in (Baras and Jiang 2004), and (Sankaranarayanan et al. 2007). Next important concept used in decision support is risk (Josang and Lo Presti 2004).

Trust models, e.g. (Wu et al. 2008), (Lifen 2008), (Ryutov et al. 2007) usually deploy merely one or two of the factors which determine trust. Present models cover more factors e.g. (Wang and Zhang. 2008). Each of these factors (e.g. reputation, recommendations, and initial trust) can be modelled as an individual component.

We propose a model that tries to integrate more of trust affecting factors, i.e. initial trust, reputation, recommendations, and trusting disposition to form a probability based phenomenal trust model.

PHENOMENAL TRUST REPRESENTATION

Trust has to be measured for applying in society models of trust. However, some simplifications and limiting presumptions must be done. For examining the trust as a behavioural pattern, some ways of representing and possibly visualizing it must be known.

Generally, trust can be quantified by a value from the interval $\langle a, b \rangle$, where a, b (a < b) are integer or real numbers. Value a represents complete distrust and value b means blind trust. Other verbal trust levels are represented by values from this interval. Without loss of generality, we will use real values from the interval $\langle 0, 1 \rangle$ as is shown in Figure 1.

Generally, mapping function which transforms verbal trust values to values from the interval $\langle 0, 1 \rangle$ is neither linear nor symmetrical.



Figure 1: Trust Value Representation

Next, we specify a phenomenal trust representation, i.e. the type of trust that the subject trusts to the phenomenon. Consider a group of *n* subjects represented as the set $S = \{s_1, s_2, ..., s_n\}$ and a group of *m* exclusive products of some kind represented as a set $P = \{p_1, p_2, ..., p_m\}$, that constitutes the phenomenon. Trust of subject x_i to product p_k is denoted as follows:

$$t_i^{\mathbf{k}} = t(s_i, p_k), \ t_i^{\mathbf{k}} \in \langle 0, 1 \rangle,$$

where: i = 1, ..., n, and k = 1, ..., m.

We use a matrix, called phenomenal trust matrix, for representation of phenomenal trust. The matrix row represents trust values of the subject to the products. The column represents trust values of subjects to the chosen product. Matrix entry -1 denotes that the subject does not know the product.

For example, phenomenal trust matrix T

$$T = \begin{pmatrix} 0.1 & 0.9 & -1 \\ 0.6 & 0 & 0.4 \\ 0.8 & 0.1 & 0.05 \end{pmatrix}$$
(1)

represents trust values of three subjects to three products. The first subject does not know the third product and the second subject completely distrusts to the second product. The total of trust values of known products Tp for single subject must hold

$$Tp = \sum_{k=1, t_i^k \neq -1}^m t_i^k \le 1$$
 (2)

Generally, phenomenal trust T_i^k of subject s_i to product p_k is function of trust forming factors

$$T_{i}^{k} = F\left(t_{i}^{k}, t_{0}^{k}, d_{i}^{k}, r_{i}^{k}, G_{i(\alpha,\beta)}\right),$$

where t_i^k is trust value of *i*-th subject to *k*-th product, $t_{0_i^k}^k$ is initial trust of *i*-th subject to *k*-th product, d_i^k is number of recommendations for *k*-th product to *i*-th subject, and r_i^k is reputation of *k*-th product by *i*-th subject considered constant over long period of time. Following must hold for reputation

$$r_i^k \in \langle 0, 1 \rangle$$
 and $\sum_{k=1, \, l_i^k \neq -1}^m r_i^k = 1$ (3)

 $G_{i(\alpha,\beta)}$, $0 \le \alpha < \beta \le 1$ is trusting disposition of subjects expressed by the probability distribution function reflecting the possible non rational aspects of trust forming.

Trust variation of *i*-th subject to *k*-th product can be expressed

$$T_i^{\mathbf{k}} = t_i^{\mathbf{k}} + \Delta t_i^{\mathbf{k}} \,,$$

where Δt_i^k is gain (loss) of phenomenal trust of *i*-th subject to *k*-th product. We propose following formula for this gain (loss)

$$\Delta t_i^k = \sqrt{t_{o_i}^k t_i^k} \quad \frac{\Delta d_i^k}{w_{d_i}} \quad \frac{r_i^k}{w_{r_i}} \frac{G_{i(\alpha,\beta)}}{w_{g_i}}, \tag{4}$$

where: $\sqrt{t_{o_i}^k t_i^k}$ is trend of trust evolution of *k*-th product by *i*-th subject with respect to initial value, Δd_i^k is relative gain (loss) of recommendations number of *k*-th product to *i*-th subject, i.e. $\left(\frac{d_i^{k[l]} - d_i^{k[l-1]}}{m}\right)$, where *l* represents *l*-th step of trust

forming process and *m* is number of products, w_{di} is weight coefficient of recommendations number of *k*-th product to *i*-th subject, w_{ri} is weight coefficient of effect of reputation of *k*-th product by *i*-th subject, and w_{ri} is weight coefficient of trusting disposition.

Thus, trust preference of *i*-th subject to *k*-th product can be now expressed

$$T_i^{\mathbf{k}} = t_i^{\mathbf{k}} + \sqrt{t_{0_i}^{\mathbf{k}} t_i^{\mathbf{k}}} \frac{\Delta d_i^{\mathbf{k}}}{w_{d_i}} \frac{r_i^{\mathbf{k}}}{w_{r_i}} \frac{G_{i(\alpha,\beta)}}{w_{g_i}}$$

Trust gain (loss) to one product is the cause of change of trust to other products to keep total of trust values Tp constant. Splitting of gain (loss), expressed in (4), to other products may be accomplished, e.g. equally, proportionally or randomly.

EXPERIMENTS

To pursue trust model behaviour we carried out series of experiments. The groups of individuals of various sizes and the groups of chosen products have been generated. The trust distribution, the initial trust matrix and reputation matrix has been chosen with uniform distribution from the interval $\langle 0, 1 \rangle$. Number of product recommendations was stepwise set up and trust forming was pursued. Next we describe the studies using five subjects and five products.

Trust Forming Study

We present the behaviour of the model on variation of phenomenal trust for six couples (subject, product), namely t_1^4 , t_2^5 , t_3^2 , t_3^3 , t_3^4 , and t_5^4 . Number of recommendation to constituent subjects, reputation values and initial trust value were generated to represent situations in everyday life. Three following tables show initial trust values (Table 1), number of recommendations in subsequent steps for selected couples (Table 2), and reputation values of products by the subjects (Table 3).

Table 1: Initial Trust Values

Initial Trust						
$t_{0_1}^4$	$t_{02}{}^5$	$t_{0_3}^2$	$t_{0_3}{}^3$	t_{03}^{4}	t_{05}^{4}	
0,05	0,01	0,15	0,59	0,04	0,01	

	Recommendation						
Step	d_1^4	d_2^{5}	d_{3}^{2}	d_3^{3}	d_{3}^{4}	d_{5}^{4}	
0	0	0	0	0	0	0	
1	3	1	2	0	1	1	
2	2	1	0	0	0	1	
3	3	1	0	0	0	2	
4	2	1	2	0	0	3	
5	4	0	0	0	3	2	

Table 2: Number of Recommendations - Stepwise

Table 3: Reputation Values of Products

Reputation						
r_1^4 r_2^5 r_3^2 r_3^3 r_3^4 r_5^4						
0,62	0,55	0,53	0,25	0,04	0,93	

Initial trusts of subjects to chosen products (for six couples) are depicted in Figure 2. The numbers of product recommendations in each step are shown in Figure 3 and product reputations in Figure 4.

Trusts evolution in subsequent steps is shown in Figure 5.



Figure 2: Initial Trust for Six Chosen Couples



Figure 3: Number of Product Recommendations



Figure 4: Product Reputations for Six Couples



Figure 5: Trust Evolution

Trust t_1^4 of subject s_1 to product p_4 changed according to the number of recommendations. Similar changes were proved in trusts t_2^{5} and t_3^{2} .

Trust of t_3^4 decreased in forth step, because subject s_3 got the same number of recommendations for product p_4 and product p_5 in this step and the reputation of product p_5 is very high (0,93) over poor reputation of product p_4 (0,04), so trust gain to product p_5 caused decrease of trust to product p_2 .

Similarly, trust t_3^3 depends on trust loss or gain to other products, even subject s_3 got no recommendation for this product. Product p_2 showed trust gain by subject s_3 in forth steps at expense of products p_3 and p_4 .

Likewise, the trust study of each subject to each product was completed. The results were in good accordance with expected behaviour.

Reputation Value Study

Next, we performed the study of reputation value influence on changes of trust to products. Five distributions of reputation values of products by subject s_1 are indicated in Table 4. Trust t_1^2 variation depending on varying reputation r_1^2 is shown in Figure 6.

Table 4: Reputation of Products by Subject s_1

	Reputation						
Case	r_1^{1}	r_1^2	r_1^{3}	r_1^{4}	r_1^{5}		
1	0,2	0,2	0,2	0,2	0,2		
2	0,16	0,35	0,17	0,16	0,16		
3	0,125	0,5	0,125	0,125	0,125		
4	0,09	0,65	0,08	0,09	0,09		
5	0,05	0,8	0,05	0,05	0,05		



Figure 6: Trust t_1^2 Variation Depending on Reputation r_1^2

High trust value is influenced by reputation strongly. On the contrary, low trust values in products fluctuate very little as shown in Figure 7.

The sensitivity of subject to a trust affecting factor is reflected by its weight coefficient. The influence of reputation weight factor on course of trust is shown in Figure 8. We can observe the possibility to reflect the subject sensitivity by the weight coefficient.







Figure 8: Trust t_1^2 Variation Depending on Reputation Weight r_1^2

Initial Trust Study

This study examines how trust to products will evolve starting with various initial values indicated in Table 5. Reputation values of products by subject s_1 are in Table 6, and Number of recommendations for subject s_1 in subsequent steps is in Table 7.

	Initial Trust						
Case	$t_{0_1}^{1}$	$t_{0_1}^2$	t_{02}^{3}	$t_{0_1}^{4}$	$t_{0_1}^{5}$		
1	0,01	0,01	0,01	0,95	0,01		
2	0,05	0,05	0,05	0,80	0,05		
3	0,08	0,08	0,08	0,65	0,09		
4	0,12	0,12	0,12	0,50	0,13		
5	0,16	0,16	0,16	0,35	0,16		

Table 6: Reputation of Products by Subject s_1

Reputation						
r_1^1 r_1^2 r_1^3 r_1^4 r_1						
0,01	0,04	0,05	0,62	0,28		

	Recommendation						
Step	d_1^{-1}	d_1^2	d_1^{3}	d_1^4	d_1^{5}		
0	0	0	0	0	0		
1	0	3	0	3	0		
2	0	1	0	2	0		
3	0	0	0	3	0		
4	0	0	0	2	0		
5	0	0	1	4	0		

Table 7: Recommendations for Products to Subject s_1

Phenomenal trust of subject s_1 to product p_4 was chosen as the example of trust forming. Trust evolution for initial trust values of subject s_1 to product p_4 is shown in Figure 9.



Figure 9: Trust t_1^4 Variation Depending on Initial Trust to_1^4

We can observe that trust changes are proportional to initial value. Further, the course of trust follows the increase and decrease of number of recommendations. To keep the total trust Tp to all known products constant, trust to other products was changed evenly.

Trusting Disposition Study

Disposition factor models the non rational aspects of a human using probability distribution function on an interval $\langle \alpha, \beta \rangle$. Its value was generated for each subject randomly and used for each product. Values $\alpha = 0.3$ and $\beta = 0.8$ were used in the study. Total ten runs were performed. Generated trusting dispositions g_i (*i*=1,...,5) of chosen subjects are shown in Table 8.

The reputation values and number of recommendations for products were the same as in the study of trust forming (Figure 4 and Figure 5).

Trust values after fifth step for selected couples are shown in Figure 10.

Table 9 and Table 10 present three experiment statistics – the arithmetic mean (AM) of trust value, the mean deviation (MD) and the standard deviation (SD) from initial trust value.

Table 8: Trusting Disposition of Subjects in Ten Runs

	Trusting Disposition							
Run	g_1	g_2	g_3	g_4	g 5			
1	0,49	0,72	0,63	0,31	0,49			
2	0,40	0,51	0,77	0,79	0,40			
3	0,39	0,38	0,65	0,59	0,39			
4	0,35	0,35	0,33	0,39	0,35			
5	0,44	0,78	0,61	0,38	0,44			
6	0,41	0,53	0,77	0,54	0,41			
7	0,59	0,53	0,32	0,30	0,59			
8	0,47	0,31	0,71	0,42	0,47			
9	0,39	0,43	0,34	0,64	0,39			
10	0,69	0,42	0,41	0,33	0,69			



Figure 10: Influence of Trusting Disposition

Table 9: Statistics of Trusting Disposition Influence 1

	Trust		
Statistic	t_1^{4}	t_2^{5}	t_{3}^{2}
AM	0,06	0,01	0,17
MD	0,0002	0,0000	0,0008
SD	0,01	0,00	0,04

Table 10: Statistics of Trusting Disposition Influence 2

	Trust		
Statistic	t_3^{3}	t_{3}^{4}	t_{5}^{4}
AM	0,58	0,04	0,01
MD	0,0002	0,0002	0,0000
SD	0,01	0,01	0,00

The effect of trusting disposition, i.e. dispersion of final trust values, grows with reputation and trust value. This is in good accordance with expected human behaviour.

CONCLUSION AND FUTURE WORK

We developed a phenomenal trust model integrating factors influencing phenomenal trust evolution. The experiments proved its behaviour to be in accordance with models considering particular factor or subset of factors in our model.

Next, we intend to pursue the collaboration with sociologist to apply the model to real cases. The model itself will be deployed in an agent based trust management model under development. Specifically we plan to study the processes of intervention, e.g. advertisement, in favour of some product.

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MODELING TECHNIQUES FOR INTEGRATION OF PROCESS SYSTEMS

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Process Systems Engineering, Hybrid modeling, integration paradox, optimization.

ABSTRACT

Increasing social, economic and environmental pressure force the process industry to look for new ways to improve the overall operation of their process systems.Since these systems are operated at different levels of decision (apparatus, plant, enterprise, etc.) integration of the different levels is expected to lead to significant improvements in system efficiency (energy, waste, costs, quality, product distribution, logistics, etc). Integration also results in increased mathematical

complexity that can not be handled with the current numerical methods. This leads inevitably to a paradox: the integrated problem needs to be decomposed again

into simpler sub-problems that are solved independently providing sub-optimal solutions. This paper will discuss why integration fails and which steps are needed to break the paradox. Focus will be on new modeling techniques for the different decision levels.

INTRODUCTION

The process industry (petrochemical-, pharmaceuticaland consumer goods industries) is an economic key sector in the world. During the last ten years, the process industry sensed an increasing pressure to reduce costs and inventories as a result of environmental, social and economic changes. The overall optimization of R&D, manufacturing and supply chain is seen as the 'holy grail' and as a complete solution to deal with these emerging changes (Grossmann (2005), Varma et al. (2007)). In the past, such process systems were relatively simple and straightforward models could be used for the optimization of the process efficiency. However, in the last decades processes became increasingly complex and are continuously subject to changes. The integration of various levels in company functions (purchasing, manufacturing, distribution and sales), distributions (markets, facilities, vendors) and decisions (strategic tactical and operational) is crucial to realize overall optimization resulting in dramatic increases in operating efficiency.

At this moment modeling and optimization at each of the levels is mostly done sequentially and this leads to the obvious question whether the optimal solutions of the individual levels are the same as the optimal solutions of the overall problem (Harjunkoski *et al.* (2008)). For the overall optimization, integration of the different levels into a monolithic structure is applied. Integration could mean

that targets are closer to their global optima, but it also encompasses the increasing complexity of the overall optimization problem. Most of these monolithic structures are NP complete problems, i.e. there is no known way to locate the solution. This conclusion leads to the integration paradox: for most industrially scaled optimization cases, the integrated problem is too complex to be solved and needs to be decomposed again into sub-problems that can be handled with the available methodologies. The integration paradox can only be broken by resolving four fundamental flaws in the integration process:

- 1. Different levels speak different languages (the models used for each of the layers differ structurally) (Wang *et al.* (2007))
- 2. There is no proper interface to communicate information between the levels (Stehphanoupoulos & Han (1996))
- 3. Methods for active re-optimization and experimental validation are not incorporated in the integrated optimization problem, making the solution insensitive to external changes (Shobrys & White (2002)) and
- 4. Numerical algorithms to deal with complex problems are far from perfect (large computational times and/or sub-optimal solutions). (Klatt & Marquardt (2008))

In this proceeding we will address the first flaw in the integration process: modeling issues. We will identify a modeling technique that is suitable for process systems integration and on the basis of two examples we will project what the capabilities of the envisaged modelin technique should be.

PROCESS MODELING

Fig. 1 shows schematically how a process system can be described by models at several levels.

At this moment, each of the levels uses different models with distinction in: mechanistic/black-box, deterministic /stochastic, distributed/lumped, discrete/continuous, linear/nonlinear, event/data-driven, etc.

The development of a modeling technique that captures the essence of each of the decision levels adequately is of crucial importance to solve the integration paradox.



Figure 1: Decomposition of a process system into several sub problems and levels, after Marquardt (Klatt & Marquardt (2008))

Several attempts were made to develop some form of uniform modeling. *CAPE and standards* Romero *et al.* (2002) used ISA standards to realize some form of uniform modeling at the higher levels and Klatt & Marquardt (2008) and Morales-Rodriguez *et al.* (2008) developed CAPE (Computer Aided Process Engineering) tools for automatic model generation for some of the levels. Their approaches, however, do not offer the possibility of integration because these models operate as stand-alone items and do not have the possibility to be connected.

Hybrid modeling

A hybrid modeling technique will do because hybrid models are constructed in such way that the structure of the model at each of the decision levels is similar, which provides the required capabilities for integration and overall optimization. The first step in a hybrid model design is to establish an Input-Output structure that describes the key variables of the process. With a basic modeling approach the process can be analyzed and a model structure can be designed on the basis of physical knowledge and process expertise. The analysis will reveal which parts are mechanistic, black-box, continuous, discrete, etc. After the analysis, the unknown parameters in the model have to be identified. Once analysis and identification are done, the model can be re-assembled into a hybrid structure (See fig. 2).

The model blocks can be connected in several ways combining parallel and serial structures. In fig. 3, a parallel and a serial two block model are shown. In a serial hybrid model, process states and fixed parameters are interchanged between the blocks while in a parallel hybrid model the blocks all require the same information.



Figure 2: Hybrid model design



Figure 3: Two-block hybrid model (left) serial model, (right) parallel model.

A hybrid modeling framework is universally applicable to each of the decision levels making integration much easier. Hybrid modeling techniques are already around

for a while, but are limited to combining discrete with continuous or phenomenological- with first-principle models. The insence for hybrid models that combine multiple representations is clearly present. *Continuous versus discrete*. We noted earlier that process systems (and control methods) are modeled in the continuous time domain as well as in the discrete event domain. The combination of these domains is called the hybrid domain. In extensive work by Baeten *et al.* (2008) a single formalism is developed that captures discrete and continuous behavior in a single modeling language. Several cases were tested, i.e. a bottle filling line, where bottles on a conveyer belt are fed from a storage tank (discrete event) while the storage tank is filled with product (continuous time domain).

Phenomenological versus first-principles

The work of van Lith *et al.* (2002) describes the development and analysis of dynamic hybrid fuzzy first principles models for process engineering applications. Such hybrid models consist of a framework of dynamic mass and energy balances (first principles) that are supplemented with fuzzy models (black-box).

EXAMPLES

In the chemical process industry are many cases that could benefit from a systematic integration of the decision levels using an extended hybrid modeling technique.

Modeling of oil refinery operations

As other heavy industries, the crude oil processing industry can be identified as an area where small increases in efficiency have a large economic impact Moulijn *et al.* (2006). The available global reserves of oil show that the available reserves for 'easy' crudes are estimated at 50 years, while the 'difficult' or shale oil reserves could supply the world for maybe 350 more years. As the easy oil becomes scarce, the need for better processing techniques becomes more urgent. World-wide research attention is drawn to new

processing techniques to increase the overall efficiency

of the crude oil processing steps. Oil refinery operations are modeled and optimized at different level of decision, and in that respect the oil refining industry is a perfect test case for an integrated hybrid modeling

methodology. Fig. 4 shows an example of an oil refinery supply chain.



Figure 4: Supply chain of an oil refinery

At nano- and micro level, physical intereactions are described (mechanistic, continuous). At meso level the temperatures, pressures, flows and compositions are modeled (mechanistic, continuous). At meso-macro level, scheduling tasks are normally evaluated: division of tasks, storage and crudes, deliveries of crudes, distribution of products, etc (discrete, linear). And at macro level, strategic decisions have to be made (heuristics). At all levels uncertainty plays a dominant role in the outcomes of the optimization.

Modeling of multi-product reactive distillation.

Reactive distillation (RD) is a successful example of process intensification. Traditionally, products where produced in reaction vessels and the products were subsequently purified in separation devices (e.g. distillation columns). Reactive distillation combines both processing steps into a single piece of equipment (See fig. 5). The advantages are numerous: smaller spaces required for the setup, reduced energy requirements, larger conversions (as removal of products shifts chemical equilibrium to the product side). Current research explores possibilities for the use of RD in a multi-product setting; a single unit is used

to produce several products (depending on the market). This poses new challenges as descriptions of such systems also require hybrid models at all levels of decision, from process control to scheduling, planning and long term strategic decisions.



Figure 5: Reactive distillation setup

In the lowest level of a multi-product reactive distillation system models that describe mass transfer, kinetics, thermodynamics and hydrodynamics are required (mechanistic, continuous, and nonlinear). These models can be used to find optimized settings for temperatures, flows, pressures, concentrations, etc (i.e. minimization of operational costs in terms of energy). At the medium levels production- and maintenance models are required that can be used to optimize production, storage and distribution of reactants and products (linear or nonlinear mixed integer models). In the higher level long-term economic models and protocols are required to optimize long-term performance of the plant, e.g. market effects (linear, stochastic and heuristics). For each level currently different model structures are used and different optimization objectives hold.

CONCLUSIONS

In this proceeding we have identified the flaws that cause the so called integration paradox. One of the flaws is the result of inconsistency in the models for each of the decision levels. Ergo, a universal modeling

technique that is applicable to all the levels could enhance the integration process significantly. Such modeling technique should incorporate process features such as mechanistic/black-box, deterministic /stochastic, distributed/lumped, discrete/continuous, linear /nonlinear, event/data driven. Hybrid modeling is such a technique. 2-Block hybrid models are currently derived for discrete/continuous systems and mechanistic/blackbox models. Extending hybrid modeling frameworks to multiple blocks, incorporating more features is a major research challenge that deserves attention.
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DESIGN EXPERIMENTS FOR THE CONSTRUCTION OF SIMULATION METAMODELS

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KEYWORDS

Metamodels; Experimental Design; Replications; Regression.

ABSTRACT

Metamodels are used as analysis tools for solving optimization problems or as surrogates used as building blocks in larger scale simulations. The metamodel replaces the simulation model by a simplified input-output relationship, frequently a mathematical function with customized parameters. The construction of a metamodel is based on the simulation results for a set of design points. In order to collect statistical information each design point may be simulated repeatedly. This paper explores the precision of the resulting metamodel based on the tradeoff between higher number of design points versus a higher number of replications at a smaller number of design points.

INTRODUCTION

Simulation models are built as replacements of real systems, and are used to assist in the analysis and optimization of those systems. The resulting model can be simulated for new inputs, giving clues about the expected behaviour of the real system under untested conditions. Furthermore, a model can be repeatedly simulated for the same inputs using different random number seeds. These replications provide valuable information about the expected uncertainties of the real system.

A simulation metamodel is a model based on a simulation model. The metamodel represents the simulation model, and thus the real system, through a simplified representation of the relationship between the inputs and outputs (Davis and Bigelow, 2003). Thus a metamodel purports only to represent the behaviour of the simulation model in an input-output sense. A straightforward method to construct a metamodel is to regress a polynomial function based on the input-output values collected from a set of design points (Kleijnen and Sargent, 2000; Santos and Santos, 2009). This polynomial function is regarded as a highly abstracted version of the reality. A simplified lowresolution representation of the system enables the simulation analyst to quickly comprehend the overall behaviour. More elaborate metamodels use radial basis functions (Jin

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et al., 2000), Bayesian approaches (Chick, 2004) or rational metamodels (Hendrickx and Dhaene, 2005). For a more realistic global response fitting, nonlinear metamodels including nonlinear regression (Santos and Nova, 2006), Kriging (Kleijnen and van Beers, 2004), and neural networks (Hurrion, 1992) are used for complex behaviours since they provide more flexible fitting.

The precision of the constructed metamodel relies heavily on the set of design points, or experimental design, used to exercise the simulation model. If those points are carefully selected, the collected results from the simulation experiments will expose the true behaviour of the system (Santos and Santos, 2008). Since simulation runs are expensive, it is desirable to infer the system's behaviour from a small number of design points. The statistical nature of the underlying model implies that a single run may not capture the mean expected behaviour of the system in regard to some entity of interest. In fact, only a number of experiments under the same input conditions expose the expected variance of a given entity. An accurate value for the statistical aspects of some entity must rely on a large number of experiments. As stated above, simulation runs are expensive and only a small number of replications can be performed at each design point.

The construction of a metamodel should require a small number of simulation runs in order to be an accessible tool. On the other hand, the information gathered must be sufficiently precise in order to produce a credible metamodel. This paper explores the precision of the resulting metamodel based on the tradeoff between higher number of design points versus a higher number of replications at a smaller number of design points. The next Section explores the construction of metamodels, specifically linear regression metamodels. The 'experimental design' Section discusses the selection of design points for the metamodel's construction. The Section entitled 'metamodel validation' is reserved for techniques to evaluate the fitting of each metamodel and to enable the comparison of previously estimated metamodels. In the 'construction tradeoff' Section the computational effort necessary to develop a metamodel is discussed. Two regions, a low variance and a high variance, of the classical M/M/1 numerical example are used to collect simulation data and built metamodels based on experimental designs using different numbers of replications

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) and design points. In the 'conclusions' Section the obtained results are analysed and summarized.

METAMODEL FITTING

The relationship between the output w and an infinite number of inputs $\mathbf{v} = v_1, v_2, \ldots$ of the real system, where some inputs may be stochastic, can be represented by a transfer function f

$$w = f(\mathbf{v}) \tag{1}$$

A simulation model of a real system can be represented by

$$y = g(\mathbf{z}, \mathbf{r}) \tag{2}$$

where y is the response, $\mathbf{z} = (z_1, \dots, z_k)^T$ is a vector of input variables and **r** is a vector of random numbers or randomly selected seeds of the pseudo-random number generators. This simulation model attempts to describe the relationship f through a few inputs. The output y of the simulation model represents the output w of the real system. The simulation program can be represented by a empirical function g.

Assume that the simulation model can be represented by a metamodel. Specifically, the general linear regression simulation metamodel

$$y_{ij} = \theta_0 + \sum_{l=1}^{q-1} \theta_l x_{il} + \epsilon_{ij}$$
(3)

Denoting ϵ_{ij} , where $\epsilon_{ij} \sim N(0, \sigma_i^2)$ with $\sigma_i > 0$, as the additive error term correspondent to the *j*-th replication of the experimental point *i* of the response. The unknown *q* metamodel parameters θ_l (l = 0, ..., q - 1) must be estimated. The explanatory variable x_l , or input *l*, may be the same as the simulation variable z_l , or a transformation of one or more variables z_l ; for example, in the M/M/1 system, the utilization factor $x_1 = z_1/z_2 = \rho$, with $z_1 = \lambda$ (arrival rate) and $z_2 = \mu$ (service rate) may be a better explanatory variable than z_1 and z_2 separately (Kleijnen, 2008). When using polynomial metamodels, the linear regression model is also applied. For example, if $\tilde{x}_{i1} = x_{i1}$ and $\tilde{x}_{i2} = x_{i1}^2$ in the regression model

$$y_{ij} = \theta_0 + \theta_1 x_{i1} + \theta_2 x_{i1}^2 + \epsilon_{ij}$$
(4)

then we obtain $y_{ij} = \theta_0 + \theta_1 \tilde{x}_{i1} + \theta_2 \tilde{x}_{i2} + \epsilon_{ij}$ which is linear in the parameters θ_0 , θ_1 , and θ_2 .

Fitting the regression metamodel to the individual responses y_{ij} is equivalent to fitting the metamodel to the averages $\bar{y}_{i.} = \sum_{j=1}^{r_i} y_{ij}/r_i$ with weights r_i ; see (Kleijnen, 1987, p. 195). Consequently, instead of problem (3), the equivalent least squares problem is considered in which the individual observations, at each design point, are replaced by their averages across simulation runs

$$\bar{y}_{i\cdot} = \theta_0 + \sum_{l=1}^{q-1} \theta_l x_{il} + \bar{\epsilon}_{i\cdot}$$
(5)

with $\bar{\epsilon}_{i} \sim N(0, \sigma_i^2/r_i)$.

In the estimation of the parameter vector $\boldsymbol{\theta}$, we considered the weighted least squares method that yield the estimator

$$\hat{\boldsymbol{\theta}} = (\mathbf{X}^T \mathbf{V}_{\bar{Y}}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{V}_{\bar{Y}}^{-1} \bar{\mathbf{Y}}$$
(6)

where $\mathbf{V}_{\bar{Y}} = \text{diag}(\sigma_1^2/r_1, \sigma_2^2/r_2, \dots, \sigma_n^2/r_n)$ is a $n \times n$ diagonal matrix, and $n \ge q = rank(\mathbf{X})$. $\mathbf{X} = (x_{il})$ denotes the $n \times q$ matrix of explanatory regression variables with x_{il} the value of explanatory variable l (i.e., input l) in design point i and $x_{i0} = 1$. If $\bar{\epsilon}_{i.} \sim N(0, \sigma^2/r_i)$ with $\sigma > 0$, then

$$\hat{\boldsymbol{\theta}} = (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{W} \bar{\mathbf{Y}}, \tag{7}$$

with $\mathbf{W} = \text{diag}(r_1, r_2, \dots, r_n)$. If the variance of the response is approximately constant for all the design points, the estimator yields

$$\hat{\boldsymbol{\theta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \bar{\mathbf{Y}}$$
(8)

In most applications the variances are unknown and $V_{\bar{Y}}$ must be estimated using the classical estimators

$$\hat{\sigma}_i^2 = \frac{1}{r_i - 1} \sum_{j=1}^{r_i} (y_{ij} - \bar{y}_{i\cdot})^2 \tag{9}$$

for estimating the *n* different variances σ_i^2 (Kleijnen and van Groenendaal, 1992). The predicted response at experimental point *i* for the resulting metamodel is given by

$$\hat{y}_{i} = \hat{\theta}_{0} + \sum_{l=1}^{q-1} \hat{\theta}_{l} x_{il}$$
(10)

EXPERIMENTAL DESIGN

The selection of input values, or experimental design, is critical to provide a good fit. An experimental design Dcorresponds to the values of the inputs over an experimental region $R \subset \mathbb{R}^q$ where the metamodel is useful. Each design point *i* in this region is designated by a specific input vector \mathbf{x}_i which must be different from every other points. These points are chosen to efficiently investigate the relationship between the design factors and the response. Assuming that the interesting features of the simulation model may belong to any part of the experimental region, the experimental design should be based on a selection of evenly distributed points throughout the region. A careful choice of an experimental design may better expose the relation between the input and the response and require less design points. In order to improve the detail of the response new points should be added (Santos and Santos, 2008) in subregions where the input-output behaviour has more interest.

Besides the selected input vector values, the response may be affected by other factors such as bias and random error (or noise). The estimation of the magnitude and distribution of the random error may be performed using replication, i.e. observing the response multiple times at the same inputs. The resulting sample means of the replicated responses have smaller variances than each individual response. To improve the detail of the response more replications (Kleijnen and Groenendaal, 1995) should be performed in high variance regions.

For each design point, a simulation run must be executed and the simulation output data collected. However, before the simulations are executed, a number of issues must be defined. These issues include the initial and final conditions, whether to perform terminating or steady-state simulations and the run length. When executing terminating simulations, that are run a pre-determined amount of time or until a certain event occurs, it may be necessary to censor the results if rare events are simulated. Otherwise, all the simulation output data should be gathered. The results obtained from steady-state simulations, that have no natural point of termination, may be biased by the warm-up period. In such cases, an initial data deletion must be performed to control the bias and reduce the estimation error in the parameters of the metamodel (Alexopoulos, 2006). Since a single mean value is gathered from each design point, simulations should not be longer than a batch or an independent replication. Then a simple mean value Y_i , at each design point *i*, is determined from gathered simulation data, for i = 1, ..., n.

METAMODEL VALIDATION

In the context of validation of simulation models, Kleijnen et al. (1998) consider a simulation model valid if the real system and the simulation model have identical real and simulated responses; see also Kleijnen et al. (2000). The validation process addresses the quality assurance of the metamodel fit. It is responsible for establishing that the metamodel closely resembles the real system and the simulation output data on which the metamodel is based. The comparison could be done using numerical statistics up to a significance level. Alternatively, the assessment could be made by using graphical plots.

The comparison can be performed with respect to the information used to build the metamodel. The available information can be analysed at three validation levels. A model adequacy relates the metamodel predicted output \hat{y}_i in Equation (10) to the simulation data used to fit the metamodel \bar{y}_i . in Equation (5). A validation with respect to the simulation model uses additional model data not directly used in the metamodel estimation, y in Equation (2). Finally, the validation with respect to the real system compares the output of the metamodel with the real data w in Equation (1). The real data may have been used to built the simulation model on which the metamodel is based.

The model adequacy compares the replicated averages \bar{y}_{i} at design point *i* used to built the metamodel with the

respective output values which the metamodel is actually able to predict. The difference between the two values, at each design point, represents the error introduced by the adjustment. To estimate the unknown parameter values of the metamodel the weighted least squares method may be used. The method consists on minimizing the error sum of squares

$$SSE(\boldsymbol{\theta}, \bar{y}) = \sum_{i=1}^{n} \frac{r_i}{\sigma_i^2} \left(\bar{y}_{i\cdot} - \theta_0 - \sum_{l=1}^{q-1} \theta_l x_{il} \right)^2 \qquad (11)$$

If the variances σ_i^2/r_i are approximately equal, assessed using a test for homogeneity of variances (Conover, 1971, page 241), then the ordinary least squares method may be used. After the parameter estimation, a goodness of fit test must be evaluated in order to assess the accuracy of the resulting metamodel. The rooted mean square error statistic

$$RMSE(\xi) = \sqrt{SSE(\hat{\theta}, \xi)/(n-q)}$$
(12)

where $\xi = \hat{y}$, also known as the fit standard error, is used as a fit statistical measure for parametric fit. A RMSE value closer to 0 indicates a better fit.

The validation with respect to the simulation model uses data collected from the simulation runs. This data can be collected at input values not used in the metamodel estimation, called predictive data. The predictive validation may also use the RMSE statistical measure taken at the new input values with the metamodel estimated with the old data, as given in Equation (12) with $\xi = y$. When using replications, each replication response value y_{ij} can be independently used as predictive data. In this case, rather than using the averages \bar{y}_{i} . in Equation (11) the errors are computed for each individual y_{ij} data not directly used in the metamodel estimation, y in Equation (2),

SSE
$$(\hat{\theta}, y) = \sum_{i=1}^{n} \sum_{j=1}^{r} \frac{r_i}{\sigma_i^2} (y_{ij} - \hat{y}_i)^2$$
 (13)

with \hat{y}_i given by Equation (10).

When data from the real system is available, the metamodel can be validated with respect to the actual data on which the simulation model was based. The RMSE, with $\xi = w$, compares the metamodel predictions at the input values from which the real data was collected, with

$$SSE(\hat{\boldsymbol{\theta}}, w) = \sum_{i=1}^{n_w} \frac{r_i}{\sigma_i^2} \left(w_i - \hat{y}_i \right)^2$$
(14)

where w_i is the real value and n_w is the number of observation available from the real system.

CONSTRUCTION TRADEOFFS

The construction of a metamodel requires a significant computational effort since a large number of simulations may be required. In fact, to obtain precise information about the behaviour of the simulation model a large number of observations may be required. Additionally, a large number of replications at each design point may be necessary to quantify the magnitude and distribution of the random error. Replications are also necessary to estimate the variance at each experimental point. If the variance is not approximately constant along the experimental region we may use estimated weighted least squares or use additional replications until $\hat{\sigma}_1^2/r_1 \simeq \ldots \simeq \hat{\sigma}_n^2/r_n$ (Kleijnen and Groenendaal, 1995; Kleijnen, 2006; Santos and Santos, 2008).

Furthermore, the length of each simulation must be determined when dealing with steady-state simulations. The length of the collected data, after the initial deletion, determines the precision of the collected data. In order to collect high precision data, longer simulation runs must be executed. However, when modeling the average behaviour of the system we may split the simulation run into batches or replications and use the observed mean response as the response value come from a large simulation. This allows us to obtain, with the same computational effort, additional statistical information that could not be obtained from one simulation run only. In short, the problem of computational effort required in metamodel building may resolve to a compromise between the number of design points and the number of replications or batches.

The aim of this paper is to check whether if the metamodel fitting is improved by an increase of the number of design points or if, on the contrary, a larger number of replications with a small number of design points produces better results. Henceforth, it is necessary to create identical conditions with respect to the computational effort used in metamodel's construction and compare the precision of the resulting matamodel. To gather meaningful conclusions it is necessary to use different experimental designs where the computational effort is successively transformed from additional replications into additional design points.

NUMERICAL EXAMPLE: M/M/1

The simple M/M/1 queuing system was simulated using AweSim version 3.0 and the metamodels built in MATLAB 6.5 using built-in and custom made routines.

We assume that customers arrive according to a Poisson process with a constant expected arrival rate, λ , and that service times follow an exponential distribution with an expected service time, $1/\mu$. The performance measure of interest is the expected waiting time in queue. The objective is to express this response as a function of the mean arrival rate (decision variable or input). We fix $1/\mu = 1$ resulting in a single input, the queue utilization factor $\rho = \lambda/\mu = \lambda$. The experiments were carried out in two different regions: a low utilization factor region, $.1 \le \rho \le .2$, and a high utilization factor region, $.8 \le \rho \le .9$. The low utilization factor experiment assumes a low and constant variance to

construct the metamodel (*low* metamodel). The high utilization factor experiment is used to built two distinct metamodels, where the parameters are estimated using the ordinary least squares (*high* metamodel) and the weighted least squares methods (*weight* metamodel).

For each of the three metamodels (*low*, *high* and *weight*) a number of equally spaced experimental designs were selected; see Table tab:design.

Table 1: Experimental designs.

design	n	r	runs
D_a	6	20	120
D_b	11	10	110
D_c	21	5	105
D_d	51	2	102
D_e	101	1	101

For each run j and for each design point i, in the low utilization factor region an initial set of 1500 observations were removed to mitigate the initial bias. The next 3000 observations were collected and averaged to produce y_{ij} . For the high utilization factor region an initial set of 6000 observations were deleted due to a longer warm-up period, and the following 3000 were collected. In fact, there were executed 20 replications at each of the 101 possible design points. Then a subset of design points and replications were selected to fulfill each experimental design requirements. For instance, the design D_a uses all 20 replications but only at design points 0.1, 0.12, 0.14, 0.16, 0.18, 0.2, while design D_e uses only one replication at each of the 101 design points. The weight estimator $r_i/\hat{\sigma}_i^2$ at each design point *i* was based on all 20 replications, even when the selected design did not use all available replications, in order to obtain the best possible estimator with the available data; see Equation (9).

Figure 1 represents the averaged mean time in queue for each experimental design in the low experimental region. As expected, as the number of replications increases, the resulting mean value gets closer to the exact value but the design points are further apart. From the figure we can infer that the variance can be assumed constant, since observations can be represented within a band of almost fixed width.

Figure 2 represents the averaged mean time in queue for each experimental design in the high experimental region. Unlike the *low* experimental region, the variance increases as the value of ρ gets closer to 0.9. Such observation leads us to introduce an estimated weighted least squares metamodel (*weight*) as well as an ordinary least squares metamodel (*high*).

The estimated metamodel values, for a second degree polynomial fitting, are depicted in Table 2. For each of these 15 fitted metamodels a set of statistical validation



Figure 1: Waiting time in queue for the *low* designs.



Figure 2: Waiting time in queue for the *high* and *weight* designs.

values were collected. Table 3 displays the adequacy statistical values of the metamodel with respect to the averaged simulation data used in the fitting process. It can be observed that, as the number of replications increases, the $RMSE(\bar{y})$ shows a steady increase as the number of design points increases and the number of replications decreases at each design point. This results from fact that the interpolation polynomial yields a null $RMSE(\bar{y})$, and as new design points are added the $RMSE(\bar{y})$ value increases as it is the sum of non-negative error values. On the other hand, as the number of replications at each design point decreases, thus the averaged value represents a rougher approximation to the true value.

A more meaningful RMSE(y) value may be based on all 20 replications of all 101 design points for any of the analysed metamodels. This RMSE(y) predictive valida-

Table 2: Estimated values for the metamodels.

	design	metamodel
	D_a	$-0.02324 x^2 + 1.379 x - 0.03117$
	D_b	$-0.9165 x^2 + 1.619 x - 0.04649$
low	D_c	$-1.285 x^2 + 1.751 x - 0.05627$
	D_d	$4.402 x^2 + 0.05655 x + 0.06582$
	D_e	$3.71 x^2 + 0.3559 x + 0.03824$
	D_a	$49.9 \ x^2 - 43.56 \ x + 7.007$
	D_b	$45.93 x^2 - 38.91 x + 5.688$
high	D_c	$-35.08 \ x^2 + 99.14 \ x - 52.91$
	D_d	$209.1 \ x^2 - 306.3 \ x + 115$
	D_e	$248.2 x^2 - 379 x + 148.4$
	D_a	$43.33 x^2 - 32.94 x + 2.713$
w eight	D_b	$182.8 x^2 - 273.4 x + 105.8$
	D_c	$93.22 x^2 - 119.7 x + 40.19$
	D_d	$280.2 x^2 - 429.7 x + 168.2$
	D_e	$191.8 x^2 - 284.2 x + 108.5$

Table 3: $RMSE(\bar{y})$ adequacy values for the metamodels.

design	low	high	weight
D_a	0.0034	0.2928	0.0389
D_b	0.0052	0.4558	0.0942
D_c	0.0071	0.5666	0.1031
D_d	0.0114	0.8770	0.1199
D_e	0.0170	1.6320	0.2383

tion values are presented in Table 4. The values obtained are very similar for each case, leading us to conclude that the number of simulation runs are fundamental to the precision of a metamodel. The amount of gathered data obtained is the important factor, whether collected as replications or as new design points.

Table 4: RMSE(y) predictive validation values for the metamodels.

design	low	high	w eight
D_a	0.0171	1.6562	0.2464
D_b	0.0172	1.6563	0.2384
D_c	0.0170	1.6641	0.2407
D_d	0.0171	1.6320	0.2378
D_e	0.0173	1.6341	0.2365

Since the M/M/1 queueing system has well known theoretical values, we used those values for the validation with respect to the real system. The results for RMSE(w) are depicted in Table 5. The results also lead us to conclude that there is no significant variation within each scenario. The concordance of the results between Table 4 and Table 5 strengthen the thesis that there is a simple tradeoff between the number of replications and the number of design points.

Table 5: RMSE(w) real system validation values for the metamodels.

design	low	high	weight
D_a	0.0030	0.3227	0.0597
D_b	0.0037	0.3517	0.0512
D_c	0.0028	0.3777	0.0446
D_d	0.0023	0.1377	0.0460
D_e	0.0029	0.1880	0.0318

CONCLUSIONS

Metamodels can be used as replacements for simulation models. The construction of a metamodel is based on the number of selected design points. At each design point a number of replications are executed in order to estimate the variance and collect other statistical values. The construction of a metamodel can become an expensive task if the number of simulation runs is large, as a result of the execution of many replications at several design points.

The precision of the metamodel is related to the number of design points and to the accuracy of the observed responses at each point. In this paper, we analysed the tradeoff between an increase in the number of design points at the expense of the number of replications at each point. Thus, by maintaining the simulation effort approximately constant the resulting precision of the fitted metamodel is evaluated as replications are replaced by new design points.

An M/M/1 example is used to exercise the proposed tradeoff since variances differ significantly from low to high utilization factors. The M/M/1 example is frequently used as work-bench for queueing systems due to the variability of expected behaviour, such as variance, as well as the availability of precise theoretical values. Furthermore, the M/M/1 theoretical values can be used as a reference for the validation of the metamodel with respect to the real system. Additional validation procedures are used to compare the metamodel with the simulation model and to check the accuracy of the metamodel.

The experiments carried out lead us to conclude that there is no significant increase in precision of the metamodel as the number of design point increases or decreases, as long as the total number of simulation runs is kept approximately constant. However, we conclude that it is preferable to have more replications and less design points, since it is possible to collect more meaningful statistical information without sacrificing the accuracy of the metamodel. The number of design points should be kept low, as far as it does not compromise the sampling of the simulation model response detail.

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PARAMETRIC ADAPTATION OF MODELS DESCRIBING STRUCTURE-DYNAMICS CONTROL PROCESSES IN COMPLEX TECHNICAL SYSTEMS (CTS)

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KEYWORDS

Complex technical systems, planning and scheduling, parametric adaptation of models

ABSTRACT

In this paper, a dynamical multiple criteria model of integrated adaptive planning and scheduling for complex technical system (CTS) is presented. Various types of CTS are used nowadays, for example: virtual enterprises, supply chains, telecommunication systems, etc. Hereafter, we mostly interpret CTS as the systems of the above-mentioned types. The adaptation control loops are explicitly integrated with the analyticalsimulation model. The mathematical approach is based on a combined application of control theory, operations research, systems analysis, and modeling and simulation theory. In particular, a scheduling problem for CTS is considered in a dynamical interpretation. New procedures of dynamic decomposition help to find the parameters value of models adaptation. The example demonstrates a general optimization scheme to be applied to the problem of competencies division between the coordinating and operating levels of CTS via parametric adaptation of models describing structure-dynamics control processes.

INTRODUCTION

In practice the processes of complex technical systems (CTS) operation are non-stationary and nonlinear. It is difficult to formalize various aspects of CTS. The CTS models have high dimensionality. There are no strict criteria of decision making for CTS managing and no a priori information about many CTS parameters. Besides, the CTS operation is always accompanied by external and internal, objective and subjective perturbation impacts. The perturbation impacts initiate the CTS structure-dynamics and predetermine a sequence of control inputs compensating the perturbation.

In other words we always come across the CTS structure dynamics in practice. There are many possible variants of CTS structure dynamics control (Ohtilev et al., 2006).

The above-mentioned CTS peculiarities do not let produce an adequate description of structure-dynamics control processes in existing and designed CTS on a basis of single-class models. That is why the concept of integrated modeling (comprehensive simulation) that was proposed by the authors can be useful here. Possible directions of its realization were considered in (Ohtilev et al., 2006, Zaychik et al., 2007). In this paper we propose new approach to the problem of parametric adaptation of models describing CTS structuredynamics control. Existence of various alternative descriptions for CTS elements and control subsystems gives an opportunity of adaptive models selection (synthesis) for program control under changing environment.

Mathematical research of control processes in CTS can be divided into three primary approaches: optimization, simulation, and heuristics. Optimization is an analysis method that determines the best possible method of designing a particular complex system. Earlier presents literature several optimization-based approaches to CTS operation planning and scheduling. For instance, (Wu et al., 1999; Ko et al., 2001; Ip et al., 2004; and Wu and Su, 2005) have applied integer programming in supporting partner selection. (Ip et al., 2004) presented a branch and bound algorithm for subcontractor selection in agile manufacturing environment.

Simulation is imitating the behaviour of one system with another. By making changes to the simulated adaptive supply chains (ASC), one expects to gain understanding of the ASC dynamics. Simulation is an ideal tool for further analyzing the performance of a proposed design derived from an optimization model. Regarding the ASC complex adaptive systems (CAS) and multi agent systems (MAS) are one of the most

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) popular simulation techniques (Swaminanthan et al. 1998; Rabelo et al., 2002). The past research on utilization of the MAS to the ASC have been mostly dealing with agent based frameworks and software architectures. It is mostly underestimated that these paradigms offer a valuable theoretical perspective on decentralized network management. (Nillson and Darley, 2006) proposed to combine CAS and MAS and to use the CAS as theoretical approach and MAS the implementation method. (Kuehnle, 2007) considers agents as a part of the complex of interrelated models for ASC planning.

Heuristics are intelligent rules that often lead to good, but not necessarily the best solutions. Heuristic approaches typically are easier to implement and require less data. However, the quality of the solution is usually unknown. Unless there is a reason that optimization cannot be used, heuristics are an inferior approach. In the ASC settings the nature based heuristics such as genetic algorithms (Huang et al., 2005) and ACO (Ant Colony Optimization) (Teich, 2003) are usually used. For instance, (Fischer et al., 2004) elaborated an approach for optimizing the selection of partners in production networks based on an ACO-algorithm.

In this paper we present a new integrated approach to planning control process in CTS. It accumulates three above-mentioned approaches.

Our investigations are based on results of the CTS adaptive control theory which is being developed now by Professor Skurihin V.I in Ukraine (Skurihin et al., 1989). The analysis of known investigations on the subject (Skurihin et al., 1989, Rastrigin, 1981, Bellman, 1972, Fleming, 1975, Nillson and Darley, 2006), confirms that the traditional tasks of CTS control should be supplemented with procedures of structural and parametric adaptation of special control software (SCS) (see fig.1 blocks 3, 7). Here the adaptive control should include the following main phases:

- parametric and structural adaptation of structure-dynamics control (SDC) models and algorithms to previous and current states of objects-inservice (SO), of control subsystems (CS), and of the environment (see fig.1, blocks 1,2,3);

 integrated planning and scheduling of CTS operation (construction of SDC programs) (blocks 4,5);

- simulation of CTS operation, according to the schedules, for different variants of control decisions in real situations and analysis of planning and scheduling simulation (blocks 6);

- structural and parametric adaptation of the schedule, control inputs, models, algorithms, and SDC programs to possible (predicted by simulation) states of SO, CS, and of the environment (blocks 7),

- realization of CTS structure-dynamics control processes (blocks 8).

To implement the proposed concept of adaptive control let us consider two groups of parameters (Skurihin et al., 1989, Rastrigin, 1980, 1981) for CTS SDC models and algorithms: *parameters that can be evaluated on the basis of real data available in CTS; parameters that can be evaluated via simulation models for different scenarios of future events*.

The adaptation procedures can be organized in two blocks (models) (Ohtilev, 2006, Skurihin et al., 1989): *external adapter of planning and scheduling models; internal adapter of planning and scheduling models.*

When the parametric adaptation of SCS does not provide simulation adequacy then the structural transformations can be needed. Two main approaches to structural model adaptation are usually distinguished (Bellman, 1972, Rastrigin, 1980, 1981). The first approach lies in the selection of a model from a given set. The model must be the most adequate to SO and CS. The second approach stands for CTS SDC model construction of elementary models (modules) in compliance with given requirements. The second approach provides more flexible adjustment of SO and CS for particular functioning conditions. However, the first one is faster and can be effective if the application knowledge base is sufficiently large.

Both approaches need active participation of system analysts and decision-makers who interact with special control software of simulation system (SIS) and consider hard-formalizing factors and dependences within the general procedure of CTS SDC program selection.

Let us consider formal statement of structural and parametric adaptation problems for CTS SDC models and after that we are going to investigate the problem of parametric adaptation for models describing CTS structure-dynamics control. Adaptation of algorithms and control software does not belong to the scope of this paper.

We have implemented the conceptual model and technology of parametric and structural adaptation of models describing CTS SDC processes via original simulation system (SIS). This simulation system consists of the following elements (Moiseev, 1974, Sowa, 2002): a) simulation models (the hierarchy of models); b) analytical models (the hierarchy of models) for a simplified (aggregated) description of objects being studied; c) informational subsystem that is a system of data bases (knowledge bases); d) control-and-coordination system for interrelation and joint use of the previous elements and interaction with the user (decision-maker).

In this paper we want to describe and to investigate concrete algorithm of parametric models adaptation via integrated modeling and simulation procedures which are realized in the SIS.



Figures 1: Conceptual model of parametric and structural adaptation (Skurihin et al., 1989)

PROBLEM STATEMENT

We assume that there are several variants of CTS SDC models inscribed in the set $\overline{\overline{M}} = \{M_1, M_2, \dots, M_W\} = \{M_\Theta, \Theta \in I\},\$ $I = \{1, ..., W\}$, moreover the vector $\vec{\beta}$ of CTS parameters includes the subvector $\vec{\beta}_0$ of fixed CTS characteristics and besides of it the subvector $\vec{w} = \parallel \vec{w}^{(1)^{\mathrm{T}}}, \ \vec{w}^{(2)^{\mathrm{T}}}, \ \vec{w}^{(3)^{\mathrm{T}}} \parallel^{\mathrm{T}}$ of parameters being adjusted through SS external/internal adapter or defined within structural adaptation. According to (Skurihin et al., 1989), these parameters can be divided into the following groups: $\vec{w}^{(1)}$ is a vector of parameters being adjusted through the internal adapter; $\vec{w}^{(2)}$ is a vector of parameters being adjusted through the external adapter; $\vec{w}^{(3)}$ is a vector of parameters being adjusted within structural adaptation of CTS SDC models.

Now we can present the modified multiplemodel multi-criteria description of CTS SDC problems:

$$\vec{J}_{\Theta}\left(\vec{x}(t), \vec{u}(t), \vec{\beta}, \vec{\xi}(t), t\right) \to \underset{\vec{u}(t) \in \Delta_{\Theta}}{\operatorname{extr}}, \qquad (1)$$

$$\Delta_{\Theta} = \{ u(t) \mid x(t) = \\ \vec{\varphi}_{\Theta} \Big(T_0, \vec{x}(T_0), \vec{x}(t), \vec{u}(t), \vec{\xi}(t), \vec{\beta}_{\Theta}, t \Big) \},$$
⁽²⁾

$$\vec{y}(t) = \vec{\psi}_{\Theta} \left(\vec{x}(t), \vec{u}(t), \vec{\xi}(t), \vec{\beta}_{\Theta}, t \right), \tag{3}$$

$$\vec{x}(T_0) \in X_0(\vec{\beta}_{\Theta}), \quad \vec{x}(T_f) \in X_f(\vec{\beta}_{\Theta}),$$
 (4)

$$\vec{u}(t) = \|\vec{u}_{pl}^{\mathsf{T}}(t), \vec{v}^{\mathsf{T}}(\vec{x}(t), t)\|^{\mathsf{T}};$$

$$\vec{u}_{pl}(t) \in Q_{\Theta}(\vec{x}(t), t);$$

$$\vec{v}(t)(\vec{x}(t), t) \in V_{\Theta}(\vec{x}(t), t);$$

$$\vec{\xi}(t) \in \Xi_{\Theta}(\vec{x}(t), t); \quad \vec{\beta}_{\Theta} \in \mathsf{B};$$

$$\vec{x}(t) \in X(\vec{\xi}(t), t);$$

$$\vec{\beta}_{\Theta} = \| \vec{\beta}_{0}^{\mathrm{T}} \vec{w}^{\mathrm{T}} \|^{\mathrm{T}}; \vec{w} = \| \vec{w}^{(1)\mathrm{T}} \vec{w}^{(2)\mathrm{T}} \vec{w}^{(3)\mathrm{T}} \|^{\mathrm{T}} .$$
(5)

The formulas define a dynamic system describing CTS structure-dynamics control processes. Here $\vec{x}(t)$ is a general state vector of the system, $\vec{y}(t)$ is a general vector of output characteristics. Then, $\vec{u}(t)$ and $\vec{v}(\vec{x}(t),t)$ are control vectors. Here $\vec{u}(t)$ represents CTS control programs (plans of CTS functioning), $\vec{v}(\vec{x}(t),t)$ is a vector of control inputs compensating perturbation impacts $\vec{\xi}(t)$). The vector $\vec{\beta}_{\Theta}$ is a general vector of CTS parameters. The vector of CTS effectiveness measures is described as (6).

$$\vec{J}_{\Theta}(\vec{x}(t), \vec{u}(t), \vec{\xi}(t), \vec{\beta}_{\Theta}, t) = \\ \| \vec{J}_{\Theta}^{(g)_{\mathrm{T}}}, \vec{J}_{\Theta}^{(o)_{\mathrm{T}}}, \vec{J}_{\Theta}^{(k)_{\mathrm{T}}}, \vec{J}_{\Theta}^{(p)_{\mathrm{T}}}, \vec{J}_{\Theta}^{(n)_{\mathrm{T}}}, \vec{J}_{\Theta}^{(e)_{\mathrm{T}}}, \vec{J}_{\Theta}^{(c)_{\mathrm{T}}}, \vec{J}_{\Theta}^{(\nu)} \|$$

$$(6)$$

Its components state control effectiveness for motion, interaction operations, channels, resources, flows, parameters, structures, and auxiliary operation operations (Ivanov et al., 2006). The indices «g», «o», «k», «p», «n», «e», «c», «v» correspond to the following models: models of order progress control $(M_{\leq g,\Theta>})$; models of operations control $(M_{\leq o,\Theta>})$; models of technological chains control $(M_{\langle k, \Theta \rangle})$; models of resources control $(M_{\leq p, \Theta >})$; models of flows control $(M_{\leq n, \Theta >})$; models of operations parameters control $(M_{\leq e, \Theta >})$; models of structures control $(M_{\leq c, \Theta \geq})$; models of auxiliary operations control $(M_{\langle v, \Theta \rangle})$. In (5) the transition function $\vec{\phi}_{\Theta}(T_0, \vec{x}(T_0), \vec{x}(t), \vec{u}(t), \vec{\xi}(t), \vec{\beta}_{\Theta}, t)$ and the output function $\vec{\Psi}_{\Theta}(\vec{x}(t), \vec{u}(t), \vec{\xi}(t), \vec{\beta}_{\Theta}, t)$ can be defined in analytical or algorithmic form within the proposed simulation system; $Q_{\Theta}(\vec{x}(t),t), \quad V_{\Theta}(\vec{x}(t),t),$

 $\Xi_{\Theta}(\vec{x}(t),t)$ are correspondingly allowable areas for program control, real-time regulation control inputs, perturbation inputs; B is a area of allowable parameters; $X(\vec{\xi}(t),t)$ is an area of allowable states of CTS structure-dynamics. Expression (4) determines end conditions for the CTS state vector $\vec{x}(t)$ at time $t = T_0$ and $t = T_f(T_0)$ is the initial time of a time interval the CTS is being investigated at, and T_f is the final time of the interval).

The problem of CTS structure-dynamics control includes tasks of three main classes: Class A problems (problems of structured analysis, problems of CTS analysis under structure-dynamics or without perturbation impacts); Class B problems [estimation monitoring (observation) problems, problems, problems of CTS structural state identification]; Class C problems (problems of control-inputs selection and problems of CTS parameters selection, i.e., multicriteria control problems for CTS structures, modes, and parameters, and multi-criteria problems of CTS structure-functional synthesis). In a general case the formal statement of CTS structure-dynamics control problem can be written as follows.

We are given: space-time, technical, and technological constraints (2)-(5) determining variants of CTS SDC at the operation phase; vector (1) of CTS effectiveness measures.

<u>We should determine</u>: $\vec{u}_{pl}(t)$, $\vec{v}(\vec{x}(t),t)$, and $\vec{\beta}_{\Theta}$ meeting the constraints (2)-(5) and returning optimal value to the general effectiveness measure $J_{\Theta}^{(ob)} = J_{\Theta}^{(ob)}(\vec{x}(t), \vec{y}(t), \vec{\beta}_{\Theta}, \vec{u}(t), \vec{\xi}(t))$.

There are two main groups of methods to be used for choice $\vec{\beta}_{\Theta}$ (Skurihin et al., 1989, Rastrigin, 1980, 1981, Bellman, 1972, Zypkin, 1969, Bryson, 1969): identification methods of parametric adaptation; simulation methods of parametric adaptation. In this paper we propose integrated procedure which helps us to find only vector $\vec{w}^{(1)}$. Others results which interrelate with parametric models adaptation are described in the book (Ohtilev et al., 2006).

ALGORITHM OF PARAMETRIC ADAPTATION OF MODELS DESCRIBING STRUCTURE-DYNAMICS CONTROL PROCESSES

The input data for the CTS planning and scheduling models adaptation is being gathered during the CTS functioning at the state S_{i-1} and is being receives to the state S_i . Thus we get formulas (Ohtilev et al., 2006,

Moiseev, 1974, Chernousko, Zak, 1985, Singh, Titli, 1978):

$$P_{H} = P_{H}\left(\vec{x}(t), \vec{u}_{pl}(t), \vec{v}\left(\vec{x}(t), \vec{\xi}\right), \vec{\xi}\right) \rightarrow \max_{\vec{u} \in \Delta}, \quad (7)$$

$$\Delta = Q(\vec{x}(t)) \times V(\vec{x}(t), \vec{\xi}, t), \quad \vec{u} = \vec{u}_{pk}(t) \times \vec{v}(\vec{x}(t), \vec{\xi})$$
(8)

where P_H is an index of CTS efficiency, $\vec{x}(t)$ is a state vector, $\vec{u}_{pk}(t)$ is the main vector of control inputs, in other words it is a control program for the CTS dynamics, \vec{v} is a vector of control inputs compensating perturbation impacts over the control program; $Q(\vec{x}(t))$ and $V(\vec{x}(t), \vec{\xi}, t)$ are the sets allowable controls $\vec{u}_{pk}(t)$ and $\vec{v}(\vec{x}(t), \vec{\xi})$ respectively; $\vec{\xi}(t)$ is a vector of perturbation impacts, where $\vec{\xi}(t) \in \Xi(\vec{x}(t), t)$.

The general efficiency measure (7) can be evaluated as a functional of $(\vec{x}(t), \vec{u}_{pl}(t), \vec{v}(\vec{x}(t), \vec{\xi}), \vec{\xi})$ via simulation experiments with the CTS operation model. Unfortunately, direct analytical expressions cannot be received. Therefore, the search for concrete control programs $(\vec{u}_{pl}(t))$ is very difficult, since the high dimensionality of the vectors $(\vec{x}(t), \vec{v}(\vec{x}(t), \vec{\xi}), \vec{\xi})$ hinder optimization through directed simulation experiments. This is why we propose the following heuristic decomposition of models (7)-(8). The decomposition is based on the structural peculiarities of these models.

The general efficiency measure of the forecasted states can be evaluated as a functional of the enumerated values via simulation experiments with the CTS operation model. In this case the following group of tasks substitutes for the initial problem of the CTS control problem (7), (8):

$$P_{H} = P_{H}\left(\vec{x}(t,\vec{\lambda}'), \vec{u}_{pl}(t,\vec{\lambda}'), \vec{v}\left(\vec{x}(t,\vec{\lambda}'), \vec{\xi}\right), \vec{\xi}\right) \to \max_{\vec{\lambda}' \in \Delta'}$$
⁽⁹⁾

$$\Delta' = \{\lambda' \mid \vec{u}_{pl}(t, \lambda') \times \vec{v} (\vec{x}(t, \lambda'), \xi) \in \mathcal{O}(\vec{x}(\vec{x}'), \xi) \in \mathcal{O}(\vec{x}'), \xi) \in \mathcal{O}(\vec{x}(\vec{x}'), \xi) \in \mathcal{O}(\vec{x}'), \xi) \in \mathcal{O}(\vec{x}(\vec{x}'), \xi) \in \mathcal{O}(\vec{x}'), \xi) \in$$

$$\begin{aligned}
\mathcal{Q}(\boldsymbol{\lambda}(\boldsymbol{\lambda})) &\stackrel{\times}{\times} \boldsymbol{\nu}(\boldsymbol{\lambda}(\boldsymbol{\lambda}), \boldsymbol{\zeta})_{\boldsymbol{\beta}} \\
&\sum_{\boldsymbol{\gamma}' \in \Gamma'} \boldsymbol{\lambda}_{\boldsymbol{\gamma}'}' J_{\boldsymbol{\gamma}'}(\vec{x}_{\boldsymbol{\gamma}'}) \rightarrow \underset{\vec{x}_{\boldsymbol{\gamma}'} \in D_{\boldsymbol{\gamma}'}(T_{f}, T_{0}, \vec{x}_{\boldsymbol{\gamma}'}(T_{0}))}{extr}, \quad (11) \\
&\sum_{\boldsymbol{\gamma}' \in \Gamma'} \boldsymbol{\lambda}_{\boldsymbol{\gamma}'}' = 1, \quad \boldsymbol{\lambda}_{\boldsymbol{\gamma}'}' \geq 0, \quad \vec{x}_{\boldsymbol{\gamma}'} = || \vec{x}^{(\boldsymbol{\gamma}')^{\mathrm{T}}} \vec{x}^{(o)^{\mathrm{T}}} ||^{\mathrm{T}}, \quad \boldsymbol{\gamma}' \in \Gamma'.
\end{aligned}$$

Here the vectors $\vec{x}_{\gamma'}(T_f)$ returning optimal values to function (16) are being searched for, while the vector $\vec{\lambda}'_{(l)}$ is fixed (l = 0, 1, 2, ... is the number of the current iteration). The set Δ' includes indices of analytical models obtained via the proposed decomposition. The received problems of mathematical programming have several important features. The search for components of the vector $\vec{x}_{\gamma'}^{(l)}$ can be fulfilled over subsets of the *attainability sets* $D_{\gamma'}(T_f, T_0, \vec{x}_{\gamma'}(T_0))$ rather than over the whole sets of allowable alternatives. The subsets include non-dominated alternatives of the enumerated models. The non-dominated alternatives can be received via the orthogonal projection of the goal sets to the *attainability sets* $D_{\gamma'}(T_f, T_0, \vec{x}_{\gamma'}(T_0))$. Each particular model include the state vector $\vec{x}^{(o)}$ of the operations model $M_{<o>}$ besides own state vectors $\vec{x}^{(g)}, \vec{x}^{(k)}, ..., \vec{x}^{(c)}$. The above-mentioned structural features of problem (11), (12) let use decomposition and overcome problem of high dimensionality.

When the vector $\vec{x}_{\gamma'}^{(l)}(T_f)$ is known, the optimal programs $\vec{u}_{pl}^{(l)}(t, \vec{\lambda}'_{(l)})$ for the CTS control can be defined within each analytical model $M_{\gamma'}, \gamma' \in \Gamma'$ via numerical methods (for example, via Krylov and Chernousko's method (Chernousko, Zak, 1985, Petrosjan, Zenkevich, 1996, Roy, 1996). The programs $\vec{u}_{pl}^{(l)}(t, \vec{\lambda}'_{(l)})$ are used for evaluation of a new approximation of the vector $\vec{\lambda}'_{(l+1)}$ in the simulation model $M_{<u>}$ describing the CTS functioning under perturbation impacts.

The problem of $\overline{\lambda}^*$ search is similar to the problem of optimal experiments design. Here elements of the vector $\overline{\lambda}'$ are endogenous variables and the efficiency measure (14) is an exogenous one. Different methods can be used for optimal design of experiments, for example the method of quickest ascent, the methods of random search. In conclusion we note that components of the vector $\overline{\lambda}'$ can define the preferable control inputs $\overline{v}(\overline{x}(t,\overline{\lambda}'),\overline{\xi})$ for compensation of mismatch of the planned trajectory of CTS dynamics with the predictable (via simulation) trajectory. Finally we propose example which illustrates one aspect of analytical-simulation procedure (9)-(12).

Structure-dynamics control processes in CTS (see formulas (1)-(5)) depend upon internal and external stochastic factors. These factors should be described through more detailed simulation models of CTS operation. These models include a deterministic component $(\vec{u}_{pl}(t), \vec{v}(\vec{x}(t), \vec{\xi}))$ describing schedules of

activities and a stochastic component $(\vec{\xi})$ describing random events (see (5)). The considered activities contributed to managerial and work and documentation. These activities could be performed at different nodes of CTS, however the sequence of activities was strictly determined within a previously obtained schedule (plan). The stochastic factors included random background and unexpected operations diverting personnel from the plan. The stochastic factors and complex interrelations of activities necessitated application of simulation. Hence, CTS optimization was to be performed via series of simulation experiments. In this situation analytical models were used to narrow parameters variation range.

This example demonstrates a general optimization scheme to be applied to the problem of competencies division between the coordinating and operating levels of CTS. The network included a coordinating level (center) and six operating levels (subsystems). Here the structural adaptation of the CTS models implied testing of different plans. The parametric adaptation of the models requires a determination of the optimal ratio of competencies (functions or tasks) expressed in man-hours. Thus, $\lambda'_{\nu'}$ (see (11)) expresses the share of

node γ' in the total amount of work. The optimization was carried out in order to reduce the plan duration. The simulation system GPSS World 4.3.5 (Minuteman Software) was used. The results presented below describe dependencies between the goal value (plan duration, hours) and the factor (competencies ratio).

The following general scheme of computations was used.

1) Problem Definition. The following global optimization problem is considered:

$$F(P_1, P_2, \dots, P_n) \to min,$$
(13)
where $PL_i \leq P_i \leq PM_i, i = 1, \dots, n.$

The parameters P_i correspond to the values $\lambda'_{\gamma'}$ in (11).

In this example the function F() expresses the plan (project) duration to be minimized.

The function (13) is defined through a simulation model. The value of the function is a probabilistic characteristic (the expectation of a plan duration) to be obtained in simulation runs.

The arguments $P_1, P_2, ..., P_n$ are model parameters (the ratio of competencies) to be varied in order to receive the minimal (the best) value of function (13).

2) Computing. The first phase. Simulation runs are being carried out. The greater total number of runs the higher is the accuracy of a solution. The run number k corresponds to a random point $(P_{1k}, P_{2k}, ..., P_{nk})$ of even distribution, where $PL_i \leq P_{ik} \leq PM_i$, i=1, ..., n. The values P_{1k} , P_{2k} , ..., P_{nk} and $F(P_{1k}, P_{2k}, ..., P_{nk})$ are stored for each k. In the GPSS World system the runs are being conducted via the "Experiment" tool of the PLUS language. The DoCommand Method is used.

3) Computing. The second phase. The functions f(s), H(s) are being approximated for the stored sample. Here f(s) is a measure of the set $Q_s = \{(q_1, q_2, ..., q_n) | F(q_1, q_2, ..., q_n) < =s, PL_i \leq q_i \leq PM_i, i=1, ..., n\},$

 $H_i(s)$ is the average value of the parameter P_i over the set Qs.

It is assumed that the smallest s^* such that $f(s^*)=0$ is the minimal value of the function $F(\bullet)$, and $P_i^*=H_i(s^*)$, i=1,...,n are the optimal values of parameters. If there holds $|F(P_1^*, P_2^*, ..., P_n^*)$ -s |>e, where e is a given level of accuracy then additional simulation runs are needed. The results of calculations are illustrated in fig. 2. Here we assume that the operating levels are unified and receive equal amounts of work, so the share of the coordinating level is to be obtained. Hence the n-tuple $(q_1, q_2, ..., q_n)$ was substituted for the scalar value q. It holds $0 \le q \le 1$. Here the left point of the graph (see fig. 2) provides the best ratio (0.23) of coordinator - executors competencies, i.e. the coordinating level receives 23% of the total amount of work.



Figures 2. Value-factor dependency, increased number of runs for a selected interval

Fig. 2 illustrates the optimization problem with nonunimodal goal function. The proposed computational scheme provides global extremum for this case.

CONCLUSIONS

The proposed approach to structure-dynamics description lets adapt heterogeneous models to the changing environment.

Dynamic decomposition of control problems helps to determine parameters of models adaptation.

There are following advantages of the proposed approach.

Joint use of diverse models (optimization, simulation, and heuristic) in the framework of poly-model systems, allows one to improve the flexibility and adaptability of planning processes in CTS, as well as to compensate the drawbacks of one class of models by the advantages of the other.

The adaptive plans (programs) of CTS functioning include transition programs as well as programs of stable CTS operation in intermediate multi-structural macro-states. One of the main opportunities of the proposed method of CTS SDC program construction is that besides the vector of program control we receive a preferable multi-structural macro-state of CTS at the end point. This is the state of CTS reliable operation in the current (forecasted) situation.

Father investigations should include an analysis of the influence of external factors upon the convergence of the planning procedures. Attributes of Pareto's set of the multi-criteria problem (see formulas (11)-(12)) will be analyzed.

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NEURAL NETWORK SIMULATION OF NITROGEN TRANSFORMATION CYCLE

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KEYWORDS

Optimal control problem with control and state constraints, adaptive critic neural network synthesis, complex system, nitrogen transformation cycle

ABSTRACT

A neural network based optimal control synthesis is presented for solving optimal control problems with control and state constraints. The optimal control problem is transcribed into a nonlinear programming problem which is implemented with adaptive critic neural network. The proposed simulation method is illustrated by the optimal control problem of nitrogen transformation cycle model. Results show that adaptive critic based systematic approach holds promise for obtaining the optimal control with control and state constraints.

INTRODUCTION

Optimal control of nonlinear systems is one of the most active subjects in control theory. There is rarely an analytical solution although several numerical computation approaches have been proposed (for example, see (Polak, 1997), (Kirk, 1998)) for solving a optimal control problem. Most of the literature that deals with numerical methods for the solution of general optimal control problems focuses on the algorithms for solving discretized problems. The basic idea of these methods is to apply nonlinear programming techniques to the resulting finite dimensional optimization problem (Buskens at al., 2000). When *Euler* integration methods are used, the recursive structure of the resulting discrete time dynamic can be exploited in computing first-order necessary condition.

In the recent years, the multi-layer feedforward neural networks have been used for obtaining numerical solutions to the optimal control problem. (Padhi at al., 2001), (Padhi et al., 2006). We have taken hyperbolic tangent sigmoid transfer function for the hidden layer and a linear transfer function for the output layer.

The paper extends adaptive critic neural network architecture proposed by (Padhi at al., 2001) to the

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) optimal control problems with control and state constraints. The paper is organized as follows. In Section 2, the optimal control problems with control and state constraints are introduced. We summarize necessary optimality conditions and give a short overview of basic result including the iterative numerical methods. Section 3 discusses discretization methods for the given optimal control problem. It also discusses a form of the resulting nonlinear programming problems. Section 4 presents a short description of adaptive critic neural network synthesis for optimal problem with state and control constraints. Section 5 consists of a nitrogen transformation model. In section 6, we apply the discussed methods to the nitrogen transformation cycle. The goal is to compare short-term and long-term strategies of assimilation of nitrogen compounds. Conclusions are presented in Section 7.

OPTIMAL CONTROL PROBLEM

We consider a nonlinear control problem subject to control and state constraints. Let $x(t) \in \mathbb{R}^n$ denote the state of a system and $u(t) \in \mathbb{R}^m$ the control in a given time interval $[t_0, t_f]$.

Optimal control problem is to minimize

$$F(x,u) = g(x(t_f)) + \int_{t_0}^{t_f} f_0(x(t), u(t)) dt \quad (1)$$

subject to

$$\begin{aligned} \dot{x}(t) &= f(x(t), u(t)), \\ x(t_0) &= x_0, \\ \psi(x(t_f)) &= 0, \\ c(x(t), u(t)) &\leq 0, \ t \in [t_0, t_f]. \end{aligned}$$

The functions $g : \mathbb{R}^n \to \mathbb{R}$, $f_0 : \mathbb{R}^{n+m} \to \mathbb{R}$, $f: \mathbb{R}^{n+m} \to \mathbb{R}^n$, $c: \mathbb{R}^{n+m} \to \mathbb{R}^q$ and $\psi: \mathbb{R}^{n+m} \to \mathbb{R}^r$, $0 \le r \le n$ are assumed to be sufficiently smooth on appropriate open sets. The theory of necessary conditions for optimal control problem of form (1) is well developed (cf. (Pontryagin at al., 1983), (Kirk, 1998)). We introduce an additional state variable

$$x_0(t) = \int_0^t f_0(x(s), u(s)) ds$$

defined by the

$$\dot{x}_0(t) = f_0(x(t), u(t)), \ x_0(0) = 0.$$

Then the augmented Hamiltonian function for problem(1) is

$$H(x,\lambda,\mu,u) = \sum_{j=0}^{n} \lambda_j f_j(x,u)$$
(2)
+
$$\sum_{j=0}^{q} \mu_j c_j(x,u)$$

where $\lambda \in R^{n+1}$ is the adjoint variable and $\mu \in R^q$ is a multiplier associated to the inequality constraints. Let (\hat{x}, \hat{u}) be an optimal solution for (1) then the necessary condition for (1) (cf. (Kirk, 1998), (Pontryagin at al., 1983)) implies that there exist a piecewise continuous and piecewise continuously differentiable adjoint function $\lambda : [t_0, t_f] \to \mathbb{R}^{n+1}$, a piecewise continuous multiplier function $\mu : [t_0, t_f] \to R^q, \ \mu(t) \ge$ 0 and a multiplier $\sigma \in \mathbb{R}^r$ satisfying

$$\begin{aligned} \dot{\lambda}_{j}(t) &= -\frac{\partial H}{\partial x_{j}}(\hat{x}(t),\lambda(t),\mu(t),\hat{u}(t)) \\ \lambda_{j}(t_{f}) &= g_{x_{j}}(\hat{x}(t_{f})) + \sigma\psi_{x_{j}}(\hat{x}(t_{f})) \\ j &= 0,\dots,n \\ \dot{\lambda}_{0}(t) &= 0 \\ 0 &= \frac{\partial H}{\partial u}(\hat{x}(t),\lambda(t),\mu(t),\hat{u}(t)). \end{aligned}$$
(3)

Herein, the subscript x or u denotes the partial derivative with respect to x or u.

DISCRETIZATION OF OPTIMAL CONTROL PROBLEM

Direct optimization methods for solving the optimal control problem are based on a suitable discretization of (1). Choose a natural number N and let $t_i \in [t_0, t_f], i =$ $0, \ldots, N$, be a equidistant mesh point with

 $t_i = t_0 + ih, i = 1, \dots, N$, where $h = \frac{t_f - t_0}{N}$. Let the vectors $x^i \in R^{n+1}, u^i \in R^m, i = 1, \dots, N$, be approximation of state variable and control variable $x(t_i)$, $u(t_i)$, respectively at the mesh point. Euler's approximation applied to the differential equations yields

$$x^{i+1} = x^i + hf(x^i, u^i), \ i = 0, \dots, N-1.$$

Choosing the optimal variable $z := (x^0, x^1, \dots, x^{N-1}, u^0, \dots, u^{N-1},) \in \mathbb{R}^{N_s}, \ N_s =$ (n+1+m)N, the optimal control problem is replaced by the following discretized control problem in the form of nonlinear programming problem with inequality constraints:

$$Minimize \ J(z) = G(x^N),$$

where

$$G(x^N) = g((x_1, \dots, x_n)^N) + x_0^N,$$

subject to

$$-x^{i+1} + x^{i} + hf(x^{i}, u^{i}) = 0, (4)$$

$$x^{0} = x(t_{0})$$

$$\psi(x^{N})) = 0,$$

$$c(x^{i}, u^{i}) \leq 0,$$

$$i = 0, \dots, N-1.$$

In a discrete-time formulation we want to find an admissible control which minimize object function (4). Let us introduce the Lagrangian function for the nonlinear optimization problem (4):

$$L(z, \lambda, \sigma, \mu) = \sum_{i=0}^{N-1} \lambda^{i+1} (-x^{i+1} + x^i + hf(x^i, u^i) + G(x^N) + \sigma\psi(x^N) + \sum_{i=0}^{N-1} \mu^i c(x^i, u^i).$$
(5)

The first order optimality conditions of Karush-Kuhn-Tucker (Polak, 1997) for the problem (4) are:

$$0 = L_{x^{i}}(s,\lambda,\mu) = \lambda^{i+1} + h\lambda^{i+1}f_{x^{i}}(x^{i},u^{i}) - \lambda^{i} + \mu^{i}c_{x^{i}}(x^{i},u^{i}), \quad (6)$$

$$i = 0, \dots, N-1,$$

$$0 = L_{x^{N}}(s,\lambda,\mu) = G_{x^{N}}(x^{N}) +$$

$$\sigma\psi_{x_{N}}(x_{N}) - \lambda^{N},$$

$$0 = L_{x^{i}}(s,\lambda,\mu) = h\lambda^{i+1}f_{x^{i}}(x^{i},u^{i})$$
(7)

$$= L_{u^{i}}(s, \lambda, \mu) = h\lambda^{i+1} f_{u^{i}}(x^{i}, u^{i}) + \mu^{i} c_{u^{i}}(x^{i}, u^{i}), \qquad (8) i = 0, \dots, N-1.$$

Eq. (6-8) represents the discrete version of necessary condition (3) for optimal control problem (1).

ADAPTIVE CRITIC NEURAL NETWORK FOR OPTIMAL CONTROL PROBLEM WITH CON-TROL AND STATE CONSTRAINTS AND FREE **TERMINAL CONDITION**

It is well known that a neural network can be used to approximate smooth time-invariant functions and uniformly time-varying function (Hornik, et al., 1989), (Sandberg, 1998). Neurons are grouped into distinct layers and interconnected according to a given architecture Fig. (1). Each connection between two neurons has a weight coefficient attached to it. The standard network structure for an approximation function is the multiplelayer perceptron (or feed forward network). The feed



Figure 1: Feed forward neural network topology with one hidden layer, v_{ji} , w_{kj} are values of connection weights, v_{j0} , w_{k0} are values of bias

forward network often has one or more hidden layers of sigmoid neurons followed by an output layer of linear neurons.

Fig. (1) shows a feed forward neural network with n_i inputs nodes one layer of n_{hl} hidden units and n_o output units. Let $in = [in_1, \ldots, in_{n_i}]$ and $out = [out_1, \ldots, out_{n_o}]$ be the input and output vectors of the network, respectively. Let $V = [v_1, \ldots, v_{n_{hl}}]$ be the matrix of synaptic weights between the input nodes and the hidden units, where $v_j = [v_{j0}, v_{j1} \ldots, v_{jn_i}], v_{j0}$ is the bias of the *j*th hidden unit, and v_{ji} is the weight that connects the *i*th input node to the *j*th hidden unit.

Let also $W = [w_1, \ldots, w_{n_o}]$ be the matrix of synaptic weights between the hidden and output units, where $w_k = [w_{k0}, w_{k1} \ldots, w_{kn_o}], w_{k0}$ is the bias of the *k*th output unit, and w_{kj} is the weight that connects the *j*th hidden units to the *k*th output unit.

The response of the jth hidden unit is given by

$$hl_j = tanh(\sum_{i=0}^{n_i} v_{ji}in_k)$$

where tanh(.) is the activation function for the hidden units. The response of the kth output unit is given by

$$out_k = \sum_{j=0}^{n_{hl}} w_{kj} hl_j.$$

Multiple layers of neurons with nonlinear transfer functions allow the network to learn nonlinear and linear relationships between input and output vectors. The number of neurons in the input and output layers is given, respectively, by the number of input and output variables in the process under investigation.

The multi-layered feed forward network shown in Fig. (2) is training using the steepest descent error backpropagation rule. Basically, it is a gradient descent, parallel



Figure 2: Architecture of adaptive critic network synthesis

distributed optimization technique to minimise the error between the network and the target output (Rumelhart at al., 1987).

In the Pontryagin's maximum principle for deriving an optimal control law, the interdependence of the state, costate and control dynamics is made clear. Indeed, the optimal control \hat{u} and multiplier $\hat{\mu}$ is given by Eq. (8), while the costate Eqs. (6 - 7) evolves backward in time and depends on the state and control. The adaptive critic neural network is based on this relationship. It consists of two network at each node: an action network the inputs of which are the current states and outputs are the corresponding control \hat{u} and multiplier $\hat{\mu}$, and the *critic* network for which the current states are inputs and current costates are outputs for normalizing the inputs and targets (zero mean and standard deviations). For detail explanation see (Rumelhart at al., 1987).

From free terminal condition $(\psi(x) \equiv 0)$ and from Eqs. (6-7) we obtain that $\lambda_0^i = -1$, for $i = N, \ldots, 0$ and $\lambda_j^N = 0$, for $j = 1, \ldots, n$. We use this observation before proceeding to the actual training of the adaptive critic neural network. The training process of the adaptive critic networks is carried out in the following steps. For $i = 1, \ldots, I$ define the sets $S_i = \{x^k \in \mathbb{R}^{n+1} : ||x^k|| < s_i\}$, where ||.|| denotes the Euclidean norm and s_i is a positive constant. The networks are trained for states within S_i . After convergence we choose $s_{i+1} > s_i$, set S_{i+1} and training the networks until i = I - 1.

The steps for training the action network are as follows: When

$$||(u^{k,a},\mu^{k,a}) - (u^{k,t},\mu^{k,t})||/||(u^{k,t},\mu^{k,t}))|| < \epsilon_a,$$

the convergence criterion for the action network training is met.

The training procedure for the critic network which expresses the relation between x^k and λ^k is as follows:

When

$$||\lambda^{k,c} - \lambda^{k,t}||/||\lambda^{k,t}|| < \epsilon_c,$$

- 1) Generate set S_i . For all $x^k \in S_i$, follow the steps below:
- (1.i) Input x^k to the action network to obtain $u^{k,a}$ and $\mu^{k,a}$.
- (1.ii) Using x^k and $u^{k,a}$ solve state equation (4) to get x^{k+1} .
- (1.iii) Input x^{k+1} to the critic network to obtain λ^{k+1} .
- (1.iv) Using x^k and λ^{k+1} solve (8) to calculate $u^{k,t}$ and $\mu^{k,t}$.
- 1) Generate set S_i . For all $x^k \in S_i$, follow the steps below:
- (1.i) Input x^k to the action network to obtain $u^{k,a}$ and $\mu^{k,a}$.
- (1.ii) Using x^k and $u^{k,a}$ solve state equation (4) to get x^{k+1} .
- (1.iii) Input x^{k+1} to the critic network to obtain λ^{k+1} .
- (1.iv) Using x^k , $u^{k,a}$, $\mu^{k,a}$ and λ^{k+1} solve (6) to calculate $\lambda^{k,t}$.
- (1.v) Input x^k to the critic network to obtain $\lambda^{k,c}$.

the convergence criterion for the critic network training is met.

Further discussion and detail explanation of this adaptive critic methods can be found in (Padhi at al., 2001), (Padhi et al., 2006).

NITROGEN TRANSFORMATION CYCLE

The aerobic transformation of nitrogen compounds (Kmet, 1996) includes:

- the decomposition of complex organic substances into simpler compounds, ammonium being the final nitrogen product,

- ammonium and nitrate oxidation,

- the assimilation of nitrates.

Specific groups of microorganisms participate in these processes. Heterotrophic bacteria (x_1) assimilates and decomposes the soluble organic nitrogen compounds DON (x_6) derived from detritus (x_5) . Ammonium (x_7) , one of the final decomposition products undergoes a biological transformation into nitrate (x_9) . This is carried out by aerobic chemoautotrophic bacteria in two stages: ammonia is first oxidized by nitrifying bacteria from the genus Nitrosomonas (x_2) into nitrites (x_8) that serve as an energy source for nitrating bacteria mainly from the genus Nitrobacter (x_3) . The resulting nitrates may be assimilated together with ammonia and soluble organic forms of nitrogen by the phytoplankton (x_4) , whereby the aerobic transformation cycle of nitrogen compounds is formed Fig. (3). The individual variables x_1, \ldots, x_9 represent nitrogen concentrations contained in the organic as well as in inorganic substances and living organisms presented in a model.

The following system of ordinary differential equa-

tions is proposed as a model for the nitrogen transformation cycle:

$$\begin{aligned} \dot{x}_{i}(t) &= x_{i}(t)U_{i}(x(t)) \\ &-x_{i}(t)E_{i}(x(t)) - x_{i}(t)M_{i}(x(t))) \\ \dot{x}_{5}(t) &= \sum_{i=1}^{4} x_{i}M_{i}(x) - K_{5}x_{5}(t) \\ \dot{x}_{6}(t) &= K_{5}x_{5}(t) - x_{1}(t)U_{1}(x(t)) + \\ & x_{4}(t)E_{4}(x(t)) - x_{4}(t)P_{6}(x(t))) \\ \dot{x}_{7}(t) &= x_{1}(t)E_{1}(x(t)) - \\ & x_{2}(t)U_{2}(x(t)) - x_{4}(t)P_{7}(x(t))) \\ \dot{x}_{8}(t) &= x_{2}(t)E_{2}(x(t)) - x_{3}(t)U_{3}(x(t)) \\ \dot{x}_{9}(t) &= x_{3}(t)E_{3}(x(t)) - x_{4}(t)P_{9}(x(t)) \end{aligned}$$

where $x_i(t)$ are the concentration of the recycling matter in microorganisms, the available nutrients and detritus, respectively (9).

$$U_i(x) = \frac{K_i x_{i+5}}{1+g_i x_{i+5}}$$
 for $i = 1, 2, 3, 4$

$$= u_1 x_6 + u_2 x_7 + u_3 x_9$$

$$U_4(x) = \frac{K_4p}{1+g_4p}$$
$$U - uptake \ rate$$

p

$$L_i(x) = \frac{a_{2i-1}U_i(x)}{1+a_{2i}U_i(x)} + 1 - \frac{a_{2i-1}}{a_{2i}}$$

$$L - excretion \ activity$$

$$\begin{array}{rcl} M_i(x) &=& g_{2i+3} + g_{2i+4}L_i(x) \\ && M - mortality \ rate \end{array}$$

$$E_i(x) = U_i(x)L_i(x) \quad for \ i = 1, 2, 3, 4$$
$$E - excretion rate$$
$$P_i(x) = \frac{K_A u_i x_i}{1 + g_A p} \quad for \ i = 6, 7, 9.$$

Three variables u = (u(1), u(2), u(3)) express the preference coefficients for update of x_6 , x_7 , x_9 . It can be expected that the phytoplankton will employ control mechanisms in such a way as to maximize its biomass over a given period T of time:

$$J(u) = \int_0^{t_f} x_4(t) dt \to max.$$

under the constraints

$$c(x, u) := b_1 U_4(x, u) + b_2 P_6(x, u) + b_3 P_9(x, u) + b_4 E_4(x, u) \leq W(I), u_i \in [0, u_{imax}] \text{ for } i = 1, 2, 3$$

The last inequality expresses the fact that amount of energy used for "living expenses" (synthesis, reduction and



Figure 3: Diagram of the compartmental system modelled by Eq. (9)

excretion of nutrients) by phytoplankton cannot exceed a certain value W(I) which depends on light intensity I(for detail explanation see (Kmet, 1996)). We introduce an additional state variable

$$x_0(t) = \int_0^t x_4(s) ds$$
 (10)

defined by the

$$\dot{x}_0(t) = x_4(t), \ x_0(0) = 0.$$

We are led to the following optimal control problems:

1) long-therm strategy:

$$Maximize \ x_0(t_f) \tag{11}$$

under the constraints

$$c(x, u) \leq W(I),$$
 (12)
 $u_i \in [0, u_{imax}] for i = 1, 2, 3.$

2) short-therm strategy:

Maximize

$$f_4(x,u) = U_4(x,u) - E_4(x,u) - M_4(x,u)$$

for all $t \in [t_0, t_f]$ under the constraints

$$\begin{aligned} c(x,u) &\leq W(I), \\ u_i &\in [0,u_{imax}] \ for \ i=1,2,3. \end{aligned}$$

Discretization of Eqs. (9 - 11) using Eqs. (6-8) and state equation (4) leads to

$$Minimize - x_0^N \tag{13}$$

subject to

$$x^{i+1} = x^i + hF(x^i, u^i)$$

$$i = 0, \dots, N - 1,$$

$$\lambda^{i} = \lambda^{i+1} + h\lambda^{i+1}F_{x^{i}}(x^{i}, u^{i}) + \mu^{i}c_{x^{i}}(x^{i}, u^{i}),$$

$$i = N - 1, \dots, 0,$$

$$\lambda^{i}_{0} = -1, i = 0, \dots, N - 1$$

$$\lambda^{N} = (-1, 0, 0, 0, 0, 0, 0, 0, 0, 0),$$
(15)

$$0 = h\lambda^{i+1}F_{u^i}(x^i, u^i)$$

$$+\mu^i c_{u^i}(x^i, u^i), \tag{16}$$

where the vector function

$$F(x, u) = (-x_4, F_1(x, u), \dots, F_9(x, u))$$

is given by Eq. (10) and by right-hand side of Eq. (9).

NUMERICAL SIMULATION

The solution of optimal control with state and control constraints using *adaptive critic neural network* and NLP methods is displayed in Figs. (4 - 8) for different initial conditions x(0) and different values of reduction coefficients b_2 and b_3 . We used values of coefficients given in Tab. (1) for numerical calculation. In the adap-



Figure 4: Adaptive critic neural network simulation of optimal control $\hat{u}(t)$ for initial condition x(0) = (0.01, 0.01, 0.02, 0.001, 0.04, 0.001, .001, 0.07, 0.01)and $b_2 < b_3$ or $b_3 < b_2$

tive critic synthesis, the critic and adaptive network were selected such that they consist of nine and four subnetworks, respectively, each having 9-27-1 structure (i.e. nine neurons in the input layer, twenty-seven neurons in the hidden layer and one neuron in the output layer). The proposed *adaptive critic neural network* is able to meet the convergence tolerance values that we choose, which led to satisfactory simulation results. Simulations, using MATLAB show that there is a very good agreement between short-term and long-term strategy and proposed neural network is able to solve nonlinear optimal control problem with state and control constraints. The optimal strategy is the following. In the presence of high ammonium concentration, the uptake of DON and nitrate is stopped. If the concentration of ammonium drops below a certain limit value, phytoplankton starts to assimilate DON or nitrate dependently on values b_2 , b_3 . If the concentration of all three forms of nitrogen are low, all of them are assimilated by phytoplankton at the maximal possible rate, e.i. $\hat{u}_i(t) = u_{imax}$ for all $t \in [t_0, t_f]$ (Fig. 4). Our results are quite similar to those obtained by (Kmet, 1996).



Figure 5: Adaptive critic neural network simulation of optimal control $\hat{u}(t)$ for initial condition x(0) = (0.1, 0.1, 0.2, 0.8, 0.4, 0.001, .001, 0.7, 1.) and $b_2 < b_3$



Figure 6: Adaptive critic neural network simulation of optimal control $\hat{u}(t)$ for initial condition x(0) = (0.1, 0.1, 0.2, 0.8, 0.4, 0.001, .001, 0.7, 1.) and $b_3 < b_2$



Figure 7: Adaptive critic neural network simulation of optimal control $\hat{u}(t)$ for initial condition x(0) = (0.1, 0.1, 0.2, 0.8, 0.4, 0.5, 0.6, 0.7, .1) and $b_2 < b_3$



Figure 8: Adaptive critic neural network simulation of optimal control $\hat{u}(t)$ for initial condition x(0) = (0.1, 0.1, 0.2, 0.8, 0.4, 0.5, 0.6, 0.7, .1) and $b_3 < b_2$

CONCLUSION

A new single network adaptive critic approach is presented for optimal control synthesis with control and state constraints. We have formulated, analysed and solved an optimal control problem related to optimal uptake of nutrient by phytoplankton. Using MATLAB, a simple simulation model based on adaptive critic neural network was constructed. Numerical simulations have shown that adaptive critic neural network is able to solve nonlinear optimal control problem with control and state constraints and it explains nutrient uptake by phytoplankton.

*

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APPENDIX

Table I. Values of the constants used in the model

$a_1 = 0.007$	$K_4 = 1.$
$a_2 = 0.0182$	$K_5 = 0.62$
$a_3 = 0.5$	$g_1 = 0.14$
$a_4 = 0.67$	$g_2 = 1.5$
$a_5 = 1.$	$g_3 = 2.0$
$a_6 = 1.39$	$g_4 = 1.5$
$a_7 = 0.66$	$g_5 = 0.8$
$a_8 = 0.67$	$g_6 = 0.4$
$b_1 = 2.92$	$g_7 = 0.2$
$b_2 = 0.4 (9.0)$	$g_8 = 0.$
$b_3 = 4.2 \ (0.4)$	$g_9 = 0.15$
$b_4 = 1.0$	$g_{10} = 0.$
W(I) = 0.51	$g_{11} = 0.1$
h=0.05	$g_{12} = 0.$
$K_1 = 19.3$	$\epsilon_a = 0.0001$
$K_2 = 8.17$	$\epsilon_c = 0.05$
$K_3 = 71.28$	$u_{1max} = 0.3$
$u_{2max} = 0.8$	$u_{3max} = 0.5$

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SOME CONSIDERATIONS CONCERNING THE MODELLING OF THE HUMAN BODY LOCOMOTOR REHABILITATION SYSTEM

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KEYWORDS

Rehabilitation model, biomechanics, gait, human body stability

ABSTRACT

In this paper the research team presents some aspects concerning the modelling of a kineto – therapeutic system for human body rehabilitation, when a locomotor disfunctionality occurred. Thus, in the first part of the paper, we analyzed theoretical aspects connected to the human body biomechanics but also to the bipedal stability. In the second part of the paper, we present the rehabilitation system model, designed to be used upon a wide range of anthropometrical dimensions. In the last part of the paper we presented the results obtained using the modelling methodologies.

INTRODUCTION

The motion actions characterizing the human body motion are subjected to some accurate objectives aiming at the normal biological functions achievement and respectively environmental adjustment. In order to produce a certain action, the muscles need to overcome by contraction a certain resistance and in this cases the muscles performing the "overcome" activity, meaning the active muscles, coexist with movements of the body muscular system, which also take part to the motion through a so called "giving in" status. These muscles have a passive effect, for example when the body is flexing, the activity is assured by the giving in contraction of the muscles in the vertebral grooves. In the dynamical activity of overcoming the muscles perform motions by shortening, while during the giving in dynamical activity, the motion is performed by the muscles extension.

The antagonist groups of muscles play an important part in determining the direction and magnitude of the motion velocity.

This fact becomes more obvious when the joints have more degrees of freedom, the motion control being thus determined by the muscular mass. The body motions are characterized by a large complexity and represent a combination of the static and dynamic behavior, thus the human factor performs partial motions of members or trunk, while other segments are fixed and serve as a support for the other areas, being called "mobile bone lever". Parts of the body muscles perform a static fixing activity for some joints, while other muscles groups develop a dynamical activity during the motion. The motion activity should be analyzed in a complex way, both in a static and a dynamic way, taking into account forces like gravity, support reaction as external forces and the muscles contraction force, ligatures resistance, elastic forces as internal forces and last but not least the forces of inertia, the resting forces and the motion forces of the mobiles the human body may be interacting with.

Another aspect to consider is the fact that the muscles static or dynamic contraction depends on the excitation degree of the motion area in the cerebral cortex, the area that sends motion impulses according to the information received on proper ways from the interoceptors, prioceptors and exteroceptors.



Fig.1. Different human body movements

The motions of the human subject are reflex acts, meaning responses of the locomotor system, in all its neuromotor complexity, to the multitude of signals arriving along the sensorial paths. Any motion, as simple as it might be, is a simple unique reflex, resulting from the connection of million reflexes, "informing" of the nervous centres, allowing the assurance of controlled and permanent coordination of motion during their performance. The accurate coordination of motions does not come all of a sudden, it is the follow up of a long series of repeated and interpreted "exercises", which determine the setting on the cerebral cortex of some temporary connections whose stability increase according to the number of repetitions and exercises stored within the central memory.

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) As a follow, the motions of the human body are performed by a series of muscles groups, which form a harmonious assembly of muscular-kinematic chains, created according to the motion particularities under the control of the cerebral cortex. The motions performed by the human body have spatial directional characteristics of the motion and of the trajectory length travelled by the body or the body segments. They may be continuous, interrupted or combined according to a certain succession. The ratio between the spatial and temporal characteristics that establish the velocity and also acceleration parameters of the motion and all these characteristics as a whole, represent the kinematic particularities of the motion: where, how much and how is the body and its segments moving, along which trajectories described by the body segments and which controlled way is the complex motion of the human body performed.

All these aspects are important to be known when we analyze the disfunctionalities of the human body locomotor system.

HUMAN BODY MOVEMENT ANALYSIS

The motions that can be performed by the human body are translations and rotations, complex and in 3D. The locomotion motions may be also cyclic or non cyclic (when the disfunctionalities occur).

The CYCLIC motions are those locomotor motions in which each part of the body returns to the initial position and then a new cycle begins, similar to the previous one. By the concept of cyclic motion we understand the totality of the motions performed by the human body and its segments, starting from a random initial position, considered as a starting point, until it reaches the next identical position. The cyclic locomotion is the result of repeating these uniform and similar cycles, also called walking or running motion units.

The NON CYCLIC motions are those locomotor motions during which there is no successive repetition of some motions cycles, such as jumps or throws, during which the body goes from an initial position to a final one and then the motion stops. This way of manifestation could be also observed in the cyclic motion with locomotor disfunctionality, those that require rehabilitation procedures in order to become cyclic motions again.

In dynamic walking, at each foot step, the system may suffer impacts and incurs on additional accelerations that influence the forward velocity (Zheng, 1984). For this reason, it was necessary to impose a set of conditions (continuity conditions) on the leg velocities so that the feet are placed on the ground carefully, without producing impact. We denote the moment of exchange of support as time t_1 , and by t_1^- and t_1^+ the times before and after the impact occurs, respectively. In normal and cyclic movement of gait process the mechanism for exchange-of-support, the angular velocities, before and after, must be identical, that is:

$$\dot{\theta}_{2i}(t_1^-) = \dot{\theta}_{1i}(t_1^+) \qquad 1 \le i \le 3 \tag{1}$$

The kinematic relations have been used and the differential problem solved to obtain the Cartesian velocities immediately before and after contact.

The foregoing derivation determined conditions for smooth exchange-of-support. In accordance, the equation of the tip of the swing leg along the *x*-axis is computed by summing a linear function with a sinusoidal function:

$$x_{21}(t) = 2V_F \left[t - \frac{1}{2\pi f} \sin\left(2\pi ft\right) \right]$$
(2)

where f is the step frequency (number of steps per unit of time).

The vertical motion, that allows the foot to be lifted off the ground, is implemented using:

$$y_{21}(t) = \frac{F_C}{2} \left[1 - \cos(2\pi f t) \right]$$
(3)

The trajectory generator is responsible for producing a motion that synchronises and coordinates the leg behaviour. In this perspective, we make sure that the swing limb arrives at the contact point when the upper body is properly centred with respect to the two lower limbs.

Energy developed into human body locomotor muscles

The amount of work done by muscles at a joint can be computed from the rate of work at the joint through time-integration. For example, the work done by the muscles at the ankle is

$$W_{AK} = \int_{t_0}^{t_1} P(M)_{AK} dt = \int_{t_0}^{t_1} T_{\frac{AK}{FT}} \cdot (\omega_{FT} - \omega_{SH}) dt \quad (4)$$

where t_o = the initial time of the movement, t_l = the final time, W_{AK} = the amount of work done by the muscles at the ankle. Equation (3) is in fact equal to the area under the muscle power-time curve. Throughout a movement, the muscle power can show both positive and negative phases. Computing the amount of work done in each phase is very important in the sense that it really gives the amount of efforts put by the muscles either concentrically or eccentrically. Integrating the muscle power-time curve for the entire phase is somewhat meaningless since the positive and negative phases cancel each other and one can only get the net work done. The muscles consume energy regardless of the mode of contraction (concentric vs. eccentric) and it is only reasonable to add all the positive and negative works done.

This can be generalized as

$$W_{JOINT}^{(+/-)} = \sum_{i} \left| \int_{t_{0}(i)}^{t_{1}(i)} P(M)_{JOINT} . dt \right|$$
(5)

where *i* = phase number, $t_o(i)$ = the initial time of the *i*-th phase, $t_i(i)$ = the final time, and $W^{(+/-)}$ = the absolute

amount of work done by muscles regardless of the contraction mode. Equation (5) is commonly used to compute the amount of **internal work** done by muscles and **the efficiency** of the **human machine**.

It is extremely important that in the procedures of conception and modelling of the rehabilitation system we perform the assessment of the energy consumption at the level of inferior members. These aspects can be emphasized in modelling by changing the kinematic and dynamic parameters like in fig.2.



Fig.2 Human leg modelling data

Following the introduction of these limits for kinematic parameters, we can get motions modelling, simple or complex, for the inferior members, modelling that will be "transferred" to the rehabilitation systems in order to be reproduced, fig.3.



Fig.3. Human body movements modelling

The simulated motions by means of the dedicated softwares lead thus to the design of the rehabilitation system in order to eliminate the locomotor dependecies on another person or equipment. At the same time this model can be a performant tool for awareness and stimulation of the human subject.

MODEL OF THE REHABILITATION SYSTEM

Dependence is defined as the state of the persons who due to some causes connected to the mitigation or loss of the physical, psychical or intelectual autonomy need assistance and/or help, which are critical in order to allow them to fulfill the current life actions. Most of the times, dependence is considered synonymous to loss of motion autonomy.

This is why sometimes the dependence on another person is possible in terms of displacement but at the same time to have some autonomy concerning the decision upon the displacement time, way or destination.

We emphasize this way the fact that dependence is not entirely opposed to autonomy but the way the involved factors approach the dependence state is very important.

All population categories may be affected by dependence. Prolonged and uncontrolled efforts, age related frailty, adjustment capacity mitigation, different physiological functions mitigation determine mobility decrease and dependence status occurrence, requiring rehabilitation actions.

Physical deficiencies are primarily caused by the locomotor hypo- or hyper- function, lack of locomotor functions balance and last but not least by the environmental factors influence.

In order to achieve the rehabilitation of the human locomotor system, we designed and structured a controlled motion module, on energetic basis, useable both in vertical position and for subjects confined to horizontal position, due to the impossibility of bipedal displacement.

For the structural and geometric achievement of the locmotor rehabilitation function system, we used **SolidWorks**.



Fig.4. Rehabilitation device model

SolidWorks represents an extremely complex design program by whose means we can generate different

structures in 3D and a multitude of simulations in order to functionally check any type of mechanisms.

The designed system with applicability on both vertical and horizontal is presented in figure 4.

Also this device is meant to perform a series of motions, which are necessary for the human locomotor system rehabilitation procedures, using the anthropometrical data of human factors and their performance limits.



Fig.5. Anthropometrical data

RESULTS AND CONCLUSIONS

The results obtained by applying different anthropometrical typo dimensions are presented in fig. 6. and fig.7.



Fig.6. Model of rehabilitation system for human height in 50% *percentile*



Fig.7. Module of rehabilitation system for human height in 75% percentile

In order to obtain a complete rehabilitation module, we considered at the same time the conception and modelling of its adjustment to the horizontal position of the human subject's bed, shown in fig.8.

The module can be easily attached or moved together with the bed, representing also an extension of its use in the locomotor rehabilitation procedures.



Fig.8. Rehabilitation module with the patient bed in horizontal position



Fig.9. Rehabilitation module in vertical position

In figures 10, 11 and 12 we presented the models of the rehabilitation device motions with respect to the previously analyzed locomotor motions.



Fig.10. Vertical position and stability of human leg

We may observe that by the very simple constructive adjustments of the rehabilitation equipment, we can simulate and respectively stimulate a series of necessary motions, we can adapt it and use it for different persons with low mobility degrees.

For the leg mobilization procedure, normally, the following movements are to be performed: flexion – extension of leg on the shank up to a global value of 70° , out of which 25° - flexion and 45° - extension; the leg abduction and adduction being performed by the complex motions of eversion and inversion with amplitude of $10^{\circ}-20^{\circ}$.

The motions of the knee joint are exclusively made in the anterior-posterior plane.

The maximum active flexion reaches 135° , while the maximum passive one 150° . The lateral legs motions or

of the entire locomotor system always represent a pathological sign or symptom.



Fig.11. Vertical position and starting gait process stimulation

Mobility examination will highlight both the passive mobility and the active one, carefully looking for possible existing joint blockage.



Fig.12. Vertical position and leg rising in gait process stimulation

All these stages of the gait process stimulation in order to rehabilitate the locomotor system are controlled by a computerized module, attached to the designed equipment (fig.9) but are initiated and monitored by special trained in motor kinetic procedures staff. Following the systematic practicing of physical exercise, respectively the use of such a device, we may notice out of the modelling values, the development within the body of some local or general effects, immediate or late, passing or lasting, which improve the human body structure and functionality. Any activity with a mobility character represents stimulation for the muscular system, whose physiological properties and physical qualities are improved.

One of the most frequent causes of the physical deficiencies is the perturbations of the muscular tonus; their correction is based on the effects of the physical exercise upon the muscle.

From educational point of view, physical exercise has a beneficial effect at any age, especially during growth period, when the motions are still not well defined, the bone growth is not yet finished, so by the correct repeating of some motions it is possible to eliminate non coherent motions and control the non coordinated ones.

As a follow, these devices can improve and develop the locomotor function being flexible, adjustable, modulated and computerized systems with multiple facilities in the rehabilitation process.

In this moment we establish a procedure to build physically this system because it is necessary to evaluate and to compare the proposed virtual model with a prototype and to find new capabilities to improve entire system and also to allow the pacients to make a variety of movements.

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HUMAN GAIT ANALYSIS FOR HIP IMPLANTED PERSONS

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KEYWORDS

Biomechanics, gait, human body implant

ABSTRACT

In this paper, the research team presents some aspects concerning the design of a methodology and a human gait analysis system for persons who suffered a locomotor disfunctionality and recovered by means of implants. Thus, in the first part of the paper we analyze theoretical aspects connected to the human body biomechanics in the process of normal gait but also those concerning the emphasis of locomotor disfunctionalities. In the second part of the paper, the recording methodology for gait dynamic parameters and the selected cases are presented. In the last part we show the results and conclusions obtained based on the proposed methodology.

INTRODUCTION

Prosthesis and/or orthesis use on neuro-motor deficient persons is absolutely necessary for many patients with bones and joints, ligament, muscular, vascular, peripherical and/or central neural deficiencies. It plays an important part within the rehabilitation measures for these patients. Prosthesis is a mean of replacing a missing anatomical segment (congenital or taken). It may be for esthetical reasons (for limbs or eye-balls), for functional mechanical purpose or using biocurrents. Orthesis is used to increase the functionality of an already existing anatomical segment, which proves to be deficient from morpho-functional point of view. It is highly important that the prosthesis or orthesis is applied in due time, as soon as possible, first on temporary basis and then on a long term basis or for the rest of the patient's life. The gait re-education is required for all forms of locomotor deficient persons.

Kineto- therapy is an important source, offering the best possible recovery to the patients. Exercises should be carefully dosaged in order to avoid the human subjects' fatigue. For better and long term efficiency they need to use relaxation techniques, simple balances and rhythmical techniques, which stimulate the vestibular system in order to obtain the general relaxation of the body muscles. The rocking-chair use reduces the muscular tonus and decreases the stiffness, as well as the rhythmical and slow roll-over the mattress have the same effect. The upside down head posture, such as the patient resting with the ventral area on a big ball produces a general relaxation by activating some medullar centers – methods that should not take too long in order to avoid the change of other physiological parameters. Thus, a series of respiratory exercises are performed with the purpose of increasing the thoracic and diaphragm mobility, while the deep and slow breaths lead to the mitigation of muscular stiffness. In order to obtain optimal results, the active and passive mobilizations must be made several times a day, thus recommending techniques of neural-muscular and prioceptive facilitation: contraction – relaxation, passive prolonged stretching.

At the same time, the exercises should be correlated with the self-caring functions because they raise the motivation and reduce some exercise abandoning manifestations.

During performing the recovery or training actions, some verbal commands even accompanied by musical rhythms are very useful, as well as big mirrors closely positioned may help to the motions regularity.

MOVEMENT ANALYSIS OF HUMAN BODY WITH GAIT AND POSTURAL DISABILITIES

During the analysis of the human motions locomotor disabilities, we started from developing a synthetic concept model, which emphasized the causes and the main milestones in measuring and assessment

In this respect we found that the locomotor disfunctionalities should be treated as substantial changes of the human body kinematics, reflected to the level of reaction forces magnitude and direction between the locomotor system and the ground.

Fig. 1 presents a synthetic model of key factors that contribute to quasi-static and dynamic postural control. This model includes feed-forward and feedback control functions. The anticipated postural disturbances, involuntarily known by the subject arise from the forces generated during the performance of voluntary motion, or in anticipation of destabilizing external forces.

This type of postural adjustment, referred to as anticipatory, involves estimation of the magnitude and direction of postural disturbance and initiation of a motor program by the central nervous system. The motor program is a set of commands that is selected based on an internal or previous model of the task to be performed. Once initiated, the motor program is executed in an open loop manner, but with the potentially processing delays inherent in feedback control. Ideally, the motor program activates the musculature that produces a set of appropriately scaled and timed pre-emptive muscle forces and joint moments that precede and deny the anticipated postural disturbance. During feedback control, a postural disturbance, the origin of which may be either internal or external, causes a change in body posture or movements. If the change in kinematics exceeds some threshold value to which the central nervous system has assigned importance, a corrective postural response will be generated.



Fig.1. Data model of human static or dynamic posture

The changes in the kinematics process stimulate visual, vestibular, and somatic-sensorial system, sensors that transmit the information to the central nervous system. Information processing by the sensorial system involves comparisons for detecting the state of the body into a desired state. In an ideal configuration, if the difference between the detected and desired states, that is, an error signal, is of sufficient magnitude, a corrective postural response consisting of muscle forces and joint moments will be executed to obtain the final response. The muscle forces and joint moments affect body kinematics, generating a new set of sensor information signals and another loop of the feedback process is initiated in this model.

EXPERIMENTAL SETUP

Within the researches concerning the hip implanted human factor gait analysis we developed a flexible and interconnected system consisting of a Kistler force plate, computerized data acquisition and processing system, high speed video camera, Fasted type with 500 frames/sec and licensed software for human gait modeling LifeMode.

The investigation conditions were established at the initial temperature, humidity and atmospheric pressure parameters, within normal limits.

The researched human subject was initially investigated and the physiological parameters such as: pulse, temperature, blood pressure, weight and height were recorded during different times of the day, when the investigations took place. The measured physiological data upon the human subject are the following: height 1,6m; weight 55,31 kg; temperature $36,3C^0$; blood pressure 14,3/7,4; pulse 70; medical diagnosis: *COTOLOIDITA* right hip (7 years old partial prosthesis); recording observations – partial help for climbing up and down in order to preserve balance.

The human subject is female, 74 years old and presents the urge of replacing the previous implanted hip prosthesis.

By help of the previous established procedure we aimed at the assessment of the dynamic parameters of the different gait variants, for which we analyze the human subject, thus accomplishing recording before the surgical intervention, immediately after and one month after, preserving the same investigation methodology.

The analysis of the X-ray images of the human subject reveals functional and position abnormalities and the decision of the medical staff was to replace the implant with a new one adjusted to the new bone configuration.



Fig.2. X-ray image of the previous implant

Due to wear and changes of the bone structure, the subject's gait was changed from the time of implant introduction until the investigation time determining an increase of the locomotor malfunction also accompanied by painful manifestations.



Fig.3. Experimental setup

Analysis processed by help of the experimental structure proposed for this research and presented in fig.3 revealed these locomotor malfunctions, allowing the development of a faster and optimized gait rehabilitation procedure.

Using this system we accomplished a series of recordings of the following gait possibilities: normal gait, added step gait, dragged gait, paced gait and backwards gait.

These recording of the gait modes were entirely performed before the implant replacement but also immediately after the surgery, when only one gait mode was possible without external help or support.

After the first recovery period (one month) we repeated the recordings of the gait modes, observing by means of the dynamic parameters analysis of the recording on the force plate, an obvious improvement.

Also the X-ray results prove the regaining hip mobility, these being corroborated with the results obtained from the software modeling and those recording by help of the experimental setup.

RESULTS AND CONCLUSIONS

The recordings were made in various times of the day before the surgery and the obtained results are presented in the following figures.

The average period of a recording was 10 sec and the motion was performed in two steps, the first one being the leg without an implant.



Fig. 4. Human subject on Kistler force plate, normal gait, two steps, starting with left leg



Fig. 5. Fz force graph, normal gait, two steps



Fig.6. Variation of Ax and COFx in the same recording



Fig.7. Surface and direction of stability field



Fig.8. Force values on Oz direction measured by 4 piezoelectric sensors of Kistler force plate



Fig. 9. The measured forces in contact time

As we may notice in the previous figures, the human subject with a 7 years old hip implant presents an important change of the normal gait, the support during gait is mainly made on the left leg, the right one being protected because it produces pain; also a strong values unbalance between the reaction forces on Oz measured by the 4 piezoelectric sensors (fig.7) and last but not least a displacement of an important part of the body weight upon the left leg joint, respectively a displacement of the gravity centre on the support surface with the tendency of falling outside it. (fig.5).

In this respect the surgery – change of hip implant – will have to correct the deficiencies and give back the mobility and motility of the locomotor system within normal limits.

Analyzing the other gait modes – added, dragged, paced and backwards we may conclude that in all cases important deviations from the normal limits occur, the subject loses balance and requires support and help during displacement, also claiming pains.

One week after the surgery, the investigations were resumed and the same set of measurements was performed in the same environmental conditions.

In the next figures, the recordings results are presented and we may notice that the displacement period is significantly longer (double), also the values of the force on Oz changed dramatically, thus emphasizing the post surgery discomfort.



Fig. 10. Fz force graph, normal gait (after 1 week) post surgery, two steps



Fig.11. Variation of Ax and COFx in the same recording post surgery



Fig.12. Stability field surface and direction for post surgery situation



Fig.13. Force values (post surgery) on Oz direction measured by 4 piezoelectric sensors of force plate



Fig. 14. The measured forces in contact time

The recorded physiological parameters during this intermediate investigation (a week after the surgery) were: weight 54,33 Kg; temperature 36,3 C⁰; blood pressure 12/4; pulse: 77; medical diagnosis: total hip prosthesis surgery using a cemented prosthesis; with the following observations: climbing up and down the force plate required partial help for preserving balance, while during normal gait the subject moves heavily using a metal frame.

After a six week recovery period, the same subject was investigated using the same experimental structure and the same environmental conditions.



Fig. 15. Human subject (post surgery) on Kistler force plate, normal gait, two steps, starting with left leg

The physiological parameters recorded after six weeks from the surgery, changed as follows: weight 56,7 Kg; temeprature $36,3C^0$; blood pressure 15,5/9 at the beginning of the recordings and 14,8/8,6 at the final of the recordings; pulse 77 and respectively 78; observations: partial help on climbing up and down the plate for balance preserving, during gait subject still needs sometimes a crutch; there are slight pains but without incurring locomotor discomfort.

Out of the recorded data at this moment we may observe a significant improvement of the subject's normal gait, due to the similarity increase between the graph of the measured reaction force and the normal graph shape.

An eloquent example proving the above stated is represented by the comparative analysis of the Oz reaction force graph during the dragged gait (because great pains were claimed and previously this type of displacement was used) in three research stages: before, immediately after and six weeks after the surgery.



Fig.16. Fz force graph, in dragged gait before surgery



Fig.17. Fz force graph, in dragged gait a week after surgery



Fig.18. Fz force graph, in dragged gait six weeks after surgery

In this respect we mention that the displacement period for this mode constantly decreased, the subject having an increased mobility and a correct balance.

Also the variations of the reaction force are constant around 540N in six weeks post surgery situation, unlike

the initial situation when this value was not constant, the variation being between 100 N and 590 N.



Fig.19. X-ray image of the replaced implant

Using these recordings we could rapidly and optimally asses the recovery stage of the human subject, who gained a better mobility and easier adopted a more balanced posture and firmer displacement.

The used experimental structures is flexible, easy to manipulate and gives the opportunity of creting an objective database for each subject, this way being able to mitigate the locomotor recovery and rehabilitation period of the implanted patients.

At this moment, using the adopted modeling and simulation methods we can accomplish rehabilitation protocols of the person with hip implant and not least assessment strategies for the post-operatory evolution.



Fig. 20. Use of the software package *OpenSim ver.1.8.1*. for simulating the post-operatory affliction

The modeling and simulation methodology of the gait afflicted by the surgical intervention is based on the inverse kinematics and dynamics applied to the models offered by the database of the software package OpenSim. Thus, starting form the complex form skeleton – tendon – muscle – joint form the software OpenSim database we introduced on this model, the measured values evaluated by the presented investigation methodology and we obtained the simulations corresponding to the recording moment (7 days, respectively 30 days after surgery). The motion equations for the muscle – skeletal system allow the calculus of the generalized coordinates accelerations resulted by applying different forces or motion limitations.

$$\begin{aligned} \ddot{\vec{a}} &= \vec{M}(\vec{a})^{-1} \left[\vec{F}(\vec{a}, \dot{\vec{a}}^2) + \vec{G}(\vec{a}) + \vec{\Gamma}(\vec{a}, \dot{\vec{a}}) + \vec{R}(\vec{a}) \vec{f}_P + \vec{S}(\vec{a}) \vec{f}_S(\vec{a}, \dot{\vec{a}}) \right] \end{aligned} \tag{1}$$

From the complementary analysis of the obtained data we can observe the similitude between the forces variation measured using the force plate and those modeled using the software package, which allows the concept of a data correlation structure.



Fig.21. Modeling of the forces action on two feet for a post-operatory patient with hip implant

This structure will allow the specialist doctor to assess and predict the subsequent post-operatory evolution of the patient and also create a fast and efficient recovery strategy.

The modeling and simulation structure, briefly presented for this case represents the subject of a more extended research, which allows the developing of an investigation-assessment-rehabilitation protocol for the hip implant patients.

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Simulation Applications in Industry
NONLINEAR MODEL FOR ROTATING MACHINE ROTOR UNDER LARGE DEFORMATION

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KEYWORDS

Rotor, Large Deformation, Nonlinear Analysis.

ABSTRACT

Reliability assessment and risk analysis of machine rotors in various overload and malfunction situations present challenge to engineers and operators. In this paper a new analytical method for evaluation of rotor under large deformation is addressed. Model is presented in general form to include also composite rotors. Presented simulation procedure is based on variational work method and has capability to account geometric nonlinearity, large for displacement, nonlinear support effect and rotor contacting other machine components. New shape functions are presented which capable to predict accurate nonlinear profile of rotor. The closed form solutions for various operating and malfunction situations are expressed. Analytical simulation results are discussed.

INTRODUCTION

Design and safety assessment of rotating machines shall be involved complete simulations of all possible overload, malfunction and accident scenarios (Adams 2001; Bloch 2006a; Brown 2005; Eshleman 2005; Fraunkner and Logan 2001; Leader 2008). Otherwise it may end up with equipment that is not safe over the full operating ranges. Rotor large deformation can be result of overloading, overspeed, resonance, whirling, accident, component failure, surge, stall, off design operation, etc and may lead to stress exceeding the safe limit (Rangwala 2005), failure of machine component, machine explosion and equipment coming apart. Each senario can cause serous damages and injuries. For reliability and safety assessment of all possible scenarios of rotating machine malfunction, it is necessary to develop an analytical method to obtain details of forces, stress and strain values for rotor under large deformation.

Now a day composite rotors (multilayer rotors) are more considered in rotating machine design. But there are limited publications for this type of rotor especially in the field of deformation and stress analysis. It is necessary to develop nonlinear stress analysis approach for composite rotors.

There are many approximate and rough analytical methods for rotor or beam analysis. One term cosine

methods are introduced and used in some publications for deflected rotors or beams. Comparison with refined Finite Element Method (F.E.M.) solution shows that one term cosine method leads to unrealistic profile and stress, in some cases, 30% higher than refined numerical results.

Some references recommended one term sine shape function for energy method which lead to simplified calculations but resulted in unrealistic high values for deformation, stress and strain. Two opposite quarter circle was also presented as shape function with geometrical conditions mainly with formulations other than energy method which is simple but inaccurate.

Large deflections of rotor entails large strain to sensitive multi-component structure and may impose excessive stress to each component of rotor which could lead to damage or even collapse. Repair processes of rotors are very expensive and time consuming. Also shut down results in lost of plant revenue for repair period. Therefore, operation of machine must be carried out with reasonable prediction and knowledge of stresses and deformations in rotor and forces to machine components.

In general analysis of rotor under large deformation requires nonlinear complex behavior simulation. It should consider changes in stiffness due to the changes in rotor geometry, nonlinear restraint of support and simulation of contact to the other machine components.

This paper offers an analytical method for assessing the effects of large deformation of rotor based on virtual work theory. It allows the investigation of numerous and different large deformation situations, provides parametric study and allows provision of curves or tables for allowable operating conditions of machine. These information and data are critical for operators for fast evaluation of rotating machine and applcation of new operating conditions or safety and reliability assessments. It is also useful for designers and rotating machine engineers for risk management, HAZOP review and vendor drawing evaluation.

Alternatives of present procedure are Finite Element Methods (F.E.M.). However, owing to the uncertainty involved in estimating support behavior and rotor embedment conditions and complex nonlinear behavior of rotor, numerical approaches need numerous sophisticated and advanced elements from several types for nonlinear effects and interactions of rotor. The appropriate use of nonlinear Finite Element Method

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(F.E.M.) for analysis of rotor, especially composite rotors, under large deformation require specialized trainings and experiences together with special software and various elements, considerable cost, time and engineering efforts. Aside from mentioned draw backs, the engineer may not gain inside the relationship between numerical results and nonlinear model. Also numerical results are not expansive and there is no provision for parametric study. Presented closed form equations in this paper are for various situations as free to deformed rotor and rotor contacting machine components. By solving these equations, unknowns can be determined and accurate rotor profile, stress and strain can be obtained. Present study is undertaken as important part of effort to develop analytical expressions for assessing the effects of large rotor deformation for normal operation as well as accidents, resonance, whirling, overloading and malfunction situations.

MODEL

Figure (1) presents model for nonlinear deformation of rotor under large deformation. This model accurately simulates rotor large deformation and includes all possible distributed and concentrated loads on rotor.



Figure 1: Model for Nonlinear Deformation of Rotor under Large Deformation.

By considering the principle of virtual work (Hall and Kabaila 1975; Rao 2007, Timoshenko and Goodier 1970; Washizu 1968) if a body is in equilibrium, the total work of all forces acting on the body in any virtual displacement vanishes. The profile of the deformed rotor is assumed as Equation (1). Variable and functions "x", " q_i " and " f_i " are coordinate along the original rotor axis, undetermined (unknown) coefficients and shape functions. With reference to physical model (Figure (1)), shape functions (" $f_i(x)$ ") are assumed smooth.

$$y(x) = \sum_{i=1}^{n} q_i f_i(x)$$
 (1)

Stated mathematically, the equilibrium condition is as Equation (2). Where "U" is the strain work and "W" is the load potential.

Equations (2) can be solved to yield the values of " q_i " that best approximate equilibrium condition. It should be noted that more terms of shape functions assumed in profile (1), closely the assumed shape resembles the true state of deformed rotor. As result, the more accurate is the approximation to the equilibrium position and the resulting internal forces and moments in machine.

$$\frac{\partial U}{\partial q_{j}} - \frac{\partial W}{\partial q_{j}} = 0 , \ j = 1 \text{ to } n$$
⁽²⁾

Total length of rotor between the points of effective anchorage supports is denoted $(L'=L+2L_A)$ and represents the portion of rotor that undergoes axial elongation as a result of loading. However, only the laterally displaced portion of rotor (*L*) undergoes bending deformation. With respect to this model the Equation (2) can be re-written as expression (3). Where " U_a ", " U_b " and " W_e " are the axial deformation strain work, bending deformation strain work and externally applied forces potential.

$$\frac{\partial U_a}{\partial q_i} + \frac{\partial U_b}{\partial q_i} - \frac{\partial W_e}{\partial q_i} = 0 , \ j = 1 \text{ to } n \qquad (3)$$

For elastic material behavior, the variation axial deformation strain work term can be expressed as Equation (4). Parameters and variables are as Equation (5) to (7). Parameter "E" and "A" are rotor elastic modulus and rotor cross section area respectively.

$$\frac{\partial U_a}{\partial q_i} = ke \frac{\partial e}{\partial q_i} \tag{4}$$

$$k = \frac{E A}{L'}, \quad L' = L + 2L_A \tag{5}$$

$$e = \widetilde{L} - L \tag{6}$$

$$\widetilde{L} = \int_{0}^{L} \sqrt{1 + \left(\frac{dy}{dx}\right)^{2}} dx$$
(7)

Variation of bending deformation strain work is expressed as Equation (8). Parameter "K" is as Equation (9). Parameter " I_{eq} " is moment of inertia of composite rotor.

$$\frac{\partial U_b}{\partial q_i} = \int_0^L K \frac{d^2 y}{dx^2} f_j'' dx \tag{8}$$

$$K = EI_{eq} \tag{9}$$

The laterally applied forces can be distributed or concentrated. The k-th concentrated lateral load " P_k " is assumed to be located at " $x=x_k$ ". Distributed lateral load "w(x)" is assumed to extended over all rotor length "L". Distributed load "P(x)" and parameter "a" and "b" are distributed load on rotor, initial and final locations of this load ("P(x)") respectively. The variation of externally applied forces potential is given by (10).

$$\frac{\partial W_e}{\partial q_j} = \int_0^L w(x) f_j(x) dx + \sum_{k=1}^m f_j(x_k) P_k$$

$$+ \int_a^b P(x) f_j(x) dx$$
(10)

With reference to Equation (5) and Figure (1), in order to determine suitable value for the length of rotor undergoing axial straining (L'), certain aspects of axial effective anchor lengths (parameter (L_A) which determined by axial support rotor interaction) shall be considered.

A rotor experiencing large lateral displacements will develop axial tension forces. It will behave like a cable. To satisfy equilibrium, this tension must be primarily balanced by the axial restraint of the support or other rotating machine or equipment shaft or rotor coupled to simulated rotor. It results in tension in rotor and coupling or shaft extension coupled to rotor. In present paper this effect has been modeled by providing for additional length of rotor (as parameter " L_A ") that extend to points of effective anchorage or fix support.

To model composite rotors, analytical expressions for the equivalent composite rotor parameters (for example composite rotor moment of inertia as parameter " I_{eq} ") shall be used in presented method. The flexural rigidity of the composite section in the elastic region can be evaluated based on the assumption that the all rotor components resist the bending as a unit with no slippage between components.

FREE TO DEFORM ROTOR

After selecting an assumed shape functions (" $f_i(x)$ " in (1)), variational expressions given by equation (3) are substituted, which are then solved by iteration to determine coefficients and to obtain equilibrium. Upon solution of the equilibrium equations, the profile of deformation, strain and stress of rotor are known. For "Free to Deform Rotor" the shape of deformed profile of rotor in the rotor deformed region (length "L") was assumed to be series of cosine curves as (11).

$$y(x) = \sum_{i=1}^{n} q_i \frac{1}{2} \left(1 - \cos\left(\frac{2(2i-1)\pi x}{L}\right) \right)$$
(11)

Equations are solved and presentd for a simple loading as uniform distributed load. Equilibrium equations can be obtained for complex and sophisticated loadings in the same manner. The equilibrium Equations (3) can be expressed as Equation (12) for uniform distributed load assumption. Coefficients " q_i " can be obtained by solving "n" equations (j=1 to n) as per expression (12). Function (y') is calculated as per Equation (13).

Solution of Equations (12) and (13) are for free to deform rotor under the uniform distributed load "w". The load "w" is the assumed equivalent uniform load of the rotor and its components. The rotor is considered to be free to deform.

$$k \left(\frac{(2j-1)\pi}{L} \right) \left(\left(\int_{0}^{L} \sqrt{1 + (y')^{2}} \, dx \right) - L \right) \left(\int_{0}^{L} \frac{\sin\left(\frac{2(2j-1)\pi x}{L}\right) y' \, dx}{\sqrt{1 + (y')^{2}}} \right) + 2K(2j-1)^{4} \frac{\pi^{4}}{L^{3}} q_{j} - \frac{1}{2} Lw = 0$$
(12)

$$y' = \frac{\pi}{L} \sum_{i=1}^{n} (2i-1)q_i \sin\left(\frac{2(2i-1)\pi x}{L}\right)$$
(13)

For an actual rotor large deformation, the rotor may not be free to deform and assumed equivalent uniform load may not be exact rotor loading situation. For some loading senarios, depending on loading and component geometry and details, uniform load assumption may result in error. For these cases proper concentrated forces and locally distributed loads shall be assigned and general solution $(w(x), P_k \text{ and } P(x) \text{ in Figure (1) and }$ Equation (10)) shall be used. Solution as (12) and (13)can also be used to check a rough clearance needed to avoid contact and accident in machine. The clearance shall be less than the calculated displacement for defined loadings. For API rotating machines at least 25% safety margin shall also be respected for calculated maximum displacement (for all possible loading from zero to trip speed) to obtain clearance.

Also solution ((12) and (13)) can be used to keep rotor under controlled stress/strain conditions. The problem can be solved by formulation ((12) and (13)) and iterating to find the maximum loadings of rotor for given allowable stress/strain. Normally the calculated stress shall be below or equal to 75% of allowable stress limit of rotor. In case of rotor contacting casing or other components, the shape function as Equation (11) is not valid and solution for rotor contacting machine components (next section) shall be used.

ROTOR CONTACTING MACHINE COMPONENT

For some assessment purposes, it is necessary to consider the effect of the rotor contacting the machine component (such as machine casing or housing). Generally contact will happen in the central portion of the rotor where rotor has maximum deformation. This solution is applicable to some abnormal situations including whirling, resonance, sever machine internal accident, overloading and tight machine clearances. After initial contact, a portion of the rotor will be in contact with machine component. For this case assumed shape to be modified to include a contact in central portion of rotor. This problem is solved by considering the half of model due to symmetric assumption. New compatible shape function shall be written and equilibrium Equation (3) for this new shape profile shall be obtained. Parameter "a" (initial location of contacting load) and other unknown coefficients (" q_i ") can be found by iteration. New shape function for rotor contacting machine component is assumed as Equation (14).

$$y(x) = \begin{cases} \sum_{i=1}^{n} \frac{1}{2} q_i \left(1 - \cos\left(\frac{(2i-1)\pi x}{a}\right) \right) 0 < x \le a \\ D_m & a < x \le \frac{L}{2} \end{cases}$$
(14)

To have a smooth profile equation $, "y(a) = D_m$ " shall be governed. This equation can be expressed as equation (15). Parameter " D_m " is initial clearance between rotor and contacted component.

$$\sum_{i=1}^{n} q_i = D_m \tag{15}$$

Assumed profile (14) is substituted to variational expression as Equation (3) for uniform distributed load. Equilibrium equations are obtained as (16). Function (y') is calculated as per (17). Variation of externally applied loads from contracted component to rotor is zero. In the other words, this load can not affect the profile of deformed rotor.

$$k \left(\frac{(2j-1)\pi}{a}\right) \left(\left(\int_{0}^{a/2} \sqrt{1+(y')^{2}} \, dx \right) - \frac{a}{2} \right) \left(\int_{0}^{a/2} \frac{\sin\left(\frac{2(2j-1)\pi x}{a}\right) y' \, dx}{\sqrt{1+(y')^{2}}} \right) + K(2j-1)^{4} \frac{\pi^{4}}{a^{3}} q_{j} - \frac{1}{4} aw = 0$$
(16)

$$y' = \frac{\pi}{a} \sum_{i=1}^{n} (2i-1)q_i \sin\left(\frac{2(2i-1)\pi x}{a}\right)$$
(17)
For $0 < x < \frac{a}{a}$

For $0 < x \le \frac{1}{2}$

Equations (15) and (16) are "n+l" equations. By solving these equation system, "n+l" unknown including "a", " q_1 ", " q_2 ",..., " q_n " will be determined..

SIMULATION RESULTS

Analytical simulation results are presented for a heavy duty special porpose centrifugal compressor rotor in refinery service. Rotor length, span, mass, diameter at coupling hub and impeller are 1880 mm, 1450 mm, 550 KG, 110 mm and 160 mm respectively. It is a rotor with five impellers (five mechanical stage compressor). Compressor nominal operating speed is 9500 rpm. Machine operating speed range is from 67% to 105% of nominal operating speed with trip at 115% of nominal operating speed. First and second critical speeds are at around 55% and 200% of machine nominal operating speed.

This rotor is simulated free to deforme to find rotor performance and clearance orders for working near first critical speed (because rotor is flexible and speed ranges are above first critical speed). Since large deformation of rotor near first critical speed is investigated, distributed variable load is respected. Rotor is modeled by equivalent uniformely distributed mass and variable distributed dynamic loading. Figure (2) presents rotor dynamic deflection vs. machine speed. This plot shows rotor deflection for machine speed from 40% to 120% of nominal operating speed including first critical speed at around 55% of nominal operating speed. Based on this plot rotor dynamic deflection in first critical speed is more than four times of rotor deflection in nominal operating condition. Presented results show importance of controlling operating speed range in variable speed rotating machine. Clearances shall be selected with

respect to maximum deflection at operating speed range. For flexible rotors (rotors which work above first critical speed) start up and speed up shall be implemented very carefully to avoid machine damage. In addition operating speed range, control system, clearances and condition monitoring shall be selected properly.



Figure 2: Rotor Deflection vs. Machine Speed for Centrifugal Compressor Rotor.

CONCLUSION

Reliability and safety assessment of rotating machines need nonlinear analysis of rotor under large deformation. The theoretical basis and analytical solution for assessing the effects of large deformation of rotor has been presented. The procedure has the capability to account nonlinear effects, large displacement geometry effects, support-rotor interaction, complicated effects of composite rotors and effects of rotor contacting the casing and other machine component. This study develops analytical procedure for fast and effective assessing the consequence of large rotor deformation in case of machine overloading, overspeed, whirling, resonance and other malfunctions or accidents. It is an effective tool for risk assessment, machine HAZOP review, operation reliability and vendor document evaluation.

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MODELLING AND SIMULATION OF CHEMICAL INDUSTRIAL REACTORS

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KEYWORDS

Modelling, Simulation, Chemical reactor, Steady-state.

ABSTRACT

The paper is focused on analysis, mathematical modelling and simulation of reactors which are used in the chemical and tanning technology. Material and energy balances are the key issues of mathematical models of chemical reactors and processes. The combination with chemical kinetics and transport effects an intellectual basis for chemical reactor design can be obtained. The contribution brings a special tanning facility – paddle tumbler which can be described as a type of rotary batch reactor and continuous-flow circulation reactor for the cyclohexane production. A mathematical dynamic model is derived and the optimal parameters were computed.

INTRODUCTION

The contribution presents a utilization of material balances with kinetic expressions for elementary chemical reaction in the phase of the reactor design. Many design engineers grope in the dark when they are facing to labyrinth of chemical and physical properties in the real world of technological plants. The paper gives simple techniques and an example how those problems can be overcome. The final derived equations of mathematical models are solved for quite simple but frequent and important chemical reactor.

The behavior of real chemical process is obviously too complex for complete mathematical analysis. We are obliged to use an approximate description which is able to deliver sufficiently accurate results. Cardinal simplifications of the mathematical description can be obtained by the following supposals:

- the process does not change its properties during the observation period,
- the relation between input and output variables of the process is linear,
- all process variables can be measured continuously and have a continuous-time trend.

In the phase of design process of many chemical, biochemical, tanning and other reactors there arise some fundamental and relevant questions. Among them, the first is: Should the reactor be batch or continuous? And subsequently: In the continuous reactor case, should it be preferred a piston flow or perfect mixing one?

For producing high-volume chemicals, flow reactors are usually preferred. The ideal piston flow reactor exactly duplicates the kinetic behavior of the ideal batch reactor. For small-volume chemicals, the economics frequently favor batch reactors. Batch reactors are used for the greater number of products, but flow reactors produce the larger volume as measured in tons.

Flow reactors are operated continuously; that is, at steady state with reactants continuously entering the vessel and with products continuously leaving. Batch reactors are operated discontinuously. A batch reaction cycle has periods for charging, reaction, and discharging. The continuous nature of a flow reactor lends itself to larger productivities and greater economies of scale than the cyclic operation of a batch reactor. The volume productivity for batch systems is identical to that of piston flow reactors and is higher than most real flow reactors. However, this volume productivity is achieved only when the reaction is actually occurring and not when the reactor is being charged or discharged, being cleaned, and so on. Within the class of flow reactors, piston flow is usually desired for reasons of productivity and selectivity.

A useful and interesting application of reactor design for chemical engineers can be seen in (Froment and Bischoff 1990), (King and Winterbottom 1998). The treatment of biochemical and polymer reaction engineering is described very extensively in (Nauman 2002), (Levenspiel 1998), (Schmidt 1998), (Smith 1956). There are emphases on numerical solutions which are needed for most practical problems in chemical reactor design. Sophisticated numerical techniques are rarely necessary. The aim is to make the techniques understandable and easily accessible and allow continued focus on the chemistry and physics of the process.

THEORETICAL BACKGROUND

Types of elementary reactions

Consider the reaction of two chemical species according to the stoichiometric equation:

$$4 + B \to P \tag{1}$$

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) This reaction is said to be homogeneous if it occurs within a single phase. It means that they take place only in the gas phase or in a single liquid phase. These reactions are said to be *elementary* if they result from a single interaction (i.e., a collision) between the molecules appearing on the left-hand side of equation (1). The rate at which collisions occur between A and B proportional molecules should be to their concentrations, a and b. Not all collisions cause a reaction, but at constant environmental conditions (e.g., temperature) some definite fraction should react. Thus, we expect

$$\Re = k[A][B] = kab \tag{2}$$

where *k* is a constant of proportionality known as the *rate constant*.

Note that the rate constant k is positive so that \Re is positive. \Re is *the rate of the reaction*, not the rate at which a particular component reacts. Components A and B are consumed by the reaction or equation (1) and thus are "formed" at a negative rate:

$$\Re_A = \Re_B = -kab \tag{3}$$

while the product P is formed at a positive rate:

$$\Re_P = +kab \tag{4}$$

The adopted sign convention supposes that the rate of a reaction is always positive. The *rate of formation of a component* is positive when the component is formed by the reaction and it is negative when the component is consumed.

First-Order Reactions

$$A \xrightarrow{k} P \quad \Re = ka$$
(5)

The rate constant k for the first-order reaction has units of $[s^{-1}]$.

Second-Order Reactions 1) One reactant:

$$2A \xrightarrow{k} P \quad \Re = ka^2 \tag{6}$$

2) Two reactants:

$$A + B \xrightarrow{k} P \quad \Re = kab \tag{7}$$

in the case of second-order reaction the rate constant k has units of $[m^3mol^{-1}s^{-1}]$.

Third-Order Reactions

In principle, there are three types of third-order reactions:

$$3A \xrightarrow{k} P \qquad \Re = ka^{3}$$

$$2A + B \xrightarrow{k} P \qquad \Re = ka^{2}b \qquad (8)$$

$$A + B + C \xrightarrow{k} P \qquad \Re = kabc$$

Types of ideal reactors

Generally, there are four basic kinds of ideal reactors:

1) The batch reactor

This is the most common type of industrial reactor. Batch reactors has no input or output of mass after the initial charging. The amounts of individual components may change due to reaction but not due to flow into or out of the reactor. The component balance for component A satisfies equation (for constant volume Vbatch reactor):

$$\frac{d(Va)}{dt} = \Re_A V \quad \Rightarrow \quad \frac{da}{dt} = \Re_A \tag{9}$$

The solution of ordinary differential equation - ODE (9) requires an initial condition: $a=a_0$ at t=0. The rate of the reaction \Re_A depends on concentration a ($\Re_A = -ka$).

2) The piston flow reactor

The piston flow reactor is continuous-flow reactor with the similar behavior as a batch reactor. It is usually visualized as a long tube in which materials stay together and react as they flow down the tube. The composition of material flowing through a piston flow reactor depends on time and also on position in the tube. The age of material at point z it t, and the composition at this point is given by the constant-volume version of the component balance for a batch reactor (9) with the substitution $t = z/\overline{u}$:

$$\overline{u}\frac{da}{dt} = \Re_A \tag{10}$$

where z is distance measured from the begin of the tube and \overline{u} is the velocity of the fluid.

3) The continuous-flow stirred tank reactor

The most important assumption is that the continuousflow stirred tank reactor is perfectly mixed. In that case there are only two possible values for concentration – the inlet flow has concentration a_{in} and everywhere else concentration a_{out} . The component balance for component A in the single reactions is:

$$Qa_{in} + \Re_A V = Qa_{out} \tag{11}$$

4) The completely segregated, continuous-flow stirred tank reactor

This type of reactor is interesting theoretically, but has

very limited practical utilization.

Obviously, no real reactor can achieve ideal state. However, it is often possible to design reactors that very closely approach ideal limits.

Temperature dependence of reactions

Chemical reactions can be isothermal or nonisothermal. In the case of isothermal reaction, the operating temperature and the rate constants are arbitrary assigned. For nonisothermal reactions, the temperature varies from the point to point in the reactor, the temperature dependence directly enters the design calculations. The rate constant k for elementary reactions is expressed by Arrhenius equation:

$$k = k_0 T^m \exp\left(\frac{-E}{RT}\right) \tag{12}$$

where parameter m=0 (or m=0.5, 1 for the special cases of reactions) depends on used theoretical model. *E* is *activation energy* and the fraction *E*/*R* is called an *activation temperature*.

A general energy balance (for a flow reactor) can be written as:

$$\rho.c_{p.}V\frac{dT}{dt} = q_{in}.\rho_{in}.c_{pin}.T_{in}$$

$$-q_{out}.\rho_{out}.c_{pout}.T_{out} - V\Delta H_{R}kc_{A} - F\alpha(T - T_{ext})$$
(13)

where term $\rho . c_p . V \frac{dT}{dt}$ is accumulation of energy, $V\Delta H_R k c_A$ is a heat generated by reaction and $F\alpha(T - T_{ext})$ is heat transferred out of reactor.

ILLUSTRATIVE EXAMPLES

The rotary batch reactor - paddle tumbler

Creation of the mathematical model of wood paddle tumbler is one of the aims of our research. The nonisothermal and non-adiabatic paddle tumbler for an enzymatic hydrolysis of chromium tannery wastes is considered. Because of simplification we can describe the paddle tumbler as a type of rotary batch reactor.

Application of paddle tumbler for an enzymatic hydrolysis in tannery has two basic reasons. Firstly, the paddle tumblers are usually used directly in the tannery wastes point of origin. Secondly, it needs only small investment to plant changes for its available utilization. Both reasons support economical and environmental aspects of the desired process.

The presented mathematical model should respect the following assumptions (Kolomaznik et al. 2006):

- Reaction mixture is intimately stirred by motion of reactor.
- Heat transfer on the both sides of wall is ideal.

- Heat of the hydrolysis reaction is inconsiderable.
- The cylinder shape reactor has radius at least 10 times greater than the thickness of wall, it means that the temperature profile can be described as "infinite plate".
- Dependence of all physical parameters of model on the temperature is negligible.

On the mentioned assumptions the quantitative mathematical model can be expressed by the following relations:

$$\frac{\partial T(x,T)}{\partial t} = a_t \frac{\partial^2 T}{\partial x^2}(c,t); 0 < x < b; t > 0 \quad (14)$$

$$m_0 c_{p0} \frac{\partial T_0(t)}{\partial t} = S\lambda \frac{\partial T}{\partial x}(0, t)$$
(15)

$$T(x,0) = T_p \tag{16}$$

$$T(b,t) = T_p \tag{17}$$

$$T(0,t) = T_0$$
(18)

$$T_0(0) = T_{0p} \tag{19}$$

A non-stationary temperature profile in the reactor wall is described by equation (14). Equation (15) describes a balance between the speed of reaction mixture temperature decrease and the heat transfer through the reactor wall. Initial conditions are expressed by equations (16) and (17). Equations (18) and (19) represent conditions of ideal heat transfer.

The time response of the reaction mixture temperature depends on the reactor wall thickness *b*, the thermal conductivity coefficient a_t , the weight of wall and reactor filling (m, m_0) and the specific heat capacity of wall and reaction mixture (c_p, c_{p0}) . The dimensional value of reaction mixture temperature $T_0(t)$ depends on its initial temperature T_{0p} and the temperature of surrounding T_p which can be identical with the initial temperature of the reactor wall (Kolomaznik et al. 2005).

From all mentioned parameters only the weight of reactor filling m_0 and its initial temperature can be changed. The weight of the reaction mixture and its initial temperature have to be chosen so that its resulting temperature do not decrease under the desired limit border (the reaction speed would be too small).

For the first approximation without nonlinearities of the temperature field in the reactor wall can be used very simple mathematical model. It is presented as a quasistationary model in the form:

$$-m_0 c_0 \frac{dT_0}{dt} = \frac{S\lambda}{b} (T_0 - T_p)$$
(20)

The solution of the model (11) is:

$$\ln\left(\frac{T_{0p} - T_p}{T_0 - T_s}\right) = \frac{S\lambda t}{bm_0 c_0}$$
(21)

The continuous-flow circulation reactor

Another presented reactor is a continuous-flow circulation reactor for the cyclohexane production. Cyclohexane, as an important base material for polyamide manufacturing, makes by catalytic hydrogenation of benzene. A large number of reaction heat transfers during hydrogenation process. Therefore, benzene and cyclohexane mixture hydrogenation proceed in continuous time circulating reactor under hydrogen excess. The presented mathematical model should respect the following conditions:

- Reaction mixture is perfectly mixed by circulation.
- The volume of reaction mixture is constant.
- All technological parameters in reactor are constant.

- Heat transfer on the both sides of wall is ideal. The hydrogenation mechanism of benzene is supposed to be a first-order reaction:

$$\underbrace{\bigcirc}_{Benzene} + 3H_2 \xrightarrow{k} \underbrace{\bigcirc}_{Cyclohexane} (22)$$

$$r_B = -k \cdot c_B$$

The material balance for the component *benzene* satisfies the following differential equation (for constant volume *V* of reactor):

$$q_v c_{Bv} = q c_B + V k c_B + V \frac{dc_B}{dt}$$
(23)

The temperature balance in the reactor satisfies the differential equation:

$$q_v . \rho_v . c_{pv} . T_v + (-\Delta H_R) V . k . c_B =$$

$$q. \rho. c_p . T + F . \alpha (T - T_x) + V . \rho. c_p \frac{dT}{dt}$$
(24)

where the relation $(-\Delta H_R)V.k.a_B$ is the heat generated by the reaction and $F.\alpha(T-T_x)$ represents the heat transfer into surroundings.

The rate constant k for elementary reactions is expressed by Arrhenius equation (12). After some mathematical manipulations the equation of the benzene concentration variation takes the form:

$$\frac{dc_B}{dt} = \frac{q_v}{V} \cdot c_{Bv} - \frac{q}{V} \cdot c_B - k_0 e^{-\frac{E}{RT}} \cdot c_B \quad (25)$$

Similarly, variation of the reaction mixture temperature in the reactor is:

$$\frac{dT}{dt} = \frac{q_v}{V} T_v + (-\Delta H_R) \cdot \frac{k \cdot c_B}{\rho \cdot c_p} - \frac{q}{V} T$$
$$-\frac{F \cdot \alpha}{V \cdot \rho \cdot c_p} (T - T_X)$$
(26)

The time response of the reaction mixture concentration depends on the input flow of the benzene, the concentration of input stream c_{Bv} , the volume of reactor filling, the specific heat capacity of reaction mixture c_p and the rate constant k. The solution of ordinary differential equation (25) requires an initial condition: $c_{Bv} = c_{B0}$ at t=0.

From all mentioned parameters the input flow stream into the reactor q_v and its initial concentration c_{Bv} can be changed.

EXPERIMENTS

The rotary batch reactor - paddle tumbler

A rotary batch reactor with diameter 1,5 m and high 1 m was used for the measuring of the temperature characteristics. Experiments took place directly in tannery industrial conditions. In the first phase 18 experiments were performed. Results of some measured variables were influenced by different factors e.g. cover leakage. From these reasons these corrupted data were not be inserted into final measurement sets. These dates were used for comparison of simulation characteristics with real values as well as for the determination of hardly measured parameters. Experiments used for comparison were carried out in a cold reactor and the filling was preheated by steam to 70-80°C. Initial parameters of are presented in Table 1.

Table 1: Initial parameters for comparative experiments

Experiment	Surrounding	Initial	Weight
number	temperature	temperature	of
	[°C]	of filling	filling
		[°C]	[kg]
experiment 14	21	80	108
experiment 17	20	80,5	155
experiment 18	20	76	155

The thermal conductivity (λ) of the wood paddle tumbler (strengthened with iron tires) was drawn from measured experimental dates. The solution of quasistationary model (14) was used. The final line (see Figure 1.) was obtained from dependence of relation

 $\ln\left(\frac{T_{0p} - T_p}{T_0 - T_s}\right)$ on the time. The thermal conductivities

were calculated by the regression analysis from measured data. Then the average value of thermal conductivity λ = 0.1031 [W/(m .K)] was calculated for the later utilization.



Figure 1: Demonstration of thermal conductivity calculation from measured dates. For experiment 18: λ =0.1036 [W/m .K]

The main problem consists in holding of the reaction mixture temperature in the range which is sufficient for a protein yield. Simulations were performed with using of the averaged thermal conductivity. The minimal reactor filling was determined as m_0 =113 [kg] upon the dependence of the reaction mixture temperature on the reactor filling.

The obtained parameters from experiments were used for simulation calculations. For the first step, mathematical model (14)-(19) was used. However, the calculated temperature profiles do not exactly follow the measured data. The difference is caused by simplifications but the main error is only in the initial phase when the heat transfer from reaction mixture into reactor wall is very high (accumulation of energy in the wall).



Figure 2: Comparison of measured (-*) and approximated (--) temperature characteristic (experiment 18).

Described rotary reactor can be for example approximated by the first order system in the form:

$$G(s) = \frac{-15}{98s + 0.8} \approx \frac{B(s)}{A(s)}$$
(27)

This approximation was obtained by a four-parameter method adopted from (Astrom 1995) applied to step responses.

The continuous-flow circulation reactor

The continuous-flow circulation reactor with V=0,5 [m³] volume was used for the simulation of the concentration and temperature characteristics. Initial input flow into the reactor was $q_v=0.0067$ [m³s⁻¹] with the initial concentration of benzene $c_{Bv}=1.9$ [kg/m³]. Initial rate constant was considered $k_0=1.616.e14$ [s⁻¹] density of mass $\rho=985$ [kg m⁻³], specific heat capacity $c_p = 4.050$ [J/kg.K], transfer heat coefficient $\alpha = 435.00$ [W/m².K], surface F=5.5 [m²], activation energy H=4.8e4 [Jmol⁻¹], initial mass temperature T_v=320 [K] and temperature of surrounding T_x=290 [K].

Steady-State Analysis Results

The dependence of the output variable upon the input in the steady-state is shown in the Figure 3. The reactor steady-state characteristics were obtained by solution of equations (12), (25) and (26). The initial conditions were computed by a standard optimization method iterative procedure.



Figure 3: Steady-state input-output behavior of the continuous-flow circulation reactor

Dynamic Analysis Results

For dynamic analysis purposes one input and one output choices were considered. Then were defined input *u* and output *y* as deviations from their steady-state values $-u(t) = q(t) - q^{s}(t)$ and $y(t) = c_{B}(t) - c_{B}^{s}(t)$.

Graphical interpretation of simulation experiments – the output y time responses to input u step changes are depicted on Figure 4.



Figure 4: The output y time responses to input u step changes, u=-0.08(1), -0.07(2), -0.05(3), 0.05(4), 0.08(5)

Model approximation

For control requirement, described continuous time circulation reactor was approximated by the second order system in the form:

$$G(s) = \frac{1.9}{71s^2 + 10s + 0.5} \approx \frac{B(s)}{A(s)}$$
(28)

The approximation was obtained by a four-parameter method adopted from (Astrom and Hagglund 1995) applied to step responses.

CONCLUSION

Developed mathematical models (especially quasistationary) enable to set up different changes of various parameters without any complex industrial experiments. A deep analysis and comparisons of experimental and simulation (computed) data were performed for verification of models. Some parameters and constants of mathematical relations had to be derived previously from measured industrial variables. Especially, the thermal conductivity of wood barrel wall had to be computed. This mathematical derivation was much simpler then performing experiments and analyzing data. After the establishing of constants and models, the minimization of the reactor filling in the first case and initial input flow or initial concentration of benzene into the reactor in the second case can be optimized. For the control requirements we have tried to approximate presented models as the first or second order inputoutput system. All computations were performed in the MATLAB+SIMULINK environment.

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RIGA AIRPORT BAGGAGE HANDLING SYSTEM SIMULATION

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KEYWORDS

Baggage handling system simulation, passenger flow forecast, development scenario estimation.

ABSTRACT

The aim of this paper is to describe the example of simulation modelling approach usage for the analysis of Riga airport baggage handling systems (BHS) work. At the first base simulation model was created using ExtendSim software. This model was based on the real passengers' measurements and documents surveys. Further, different scenarios of BHS development were implemented. Different characteristics of BHS were estimated for the use of developed model. Conclusions the and recommendations are based on the results of the investigation.

INTRODUCTION

During last years air transport becomes more and more popular as a means of traveling. Few facts concerns us about that. The number of passengers in 2007 reached 650 million peoples. The turnover of air transport is 260 billions per year. The air transport network is 15 millions kilometers and includes 10000 airports all over the world.

Air transport branch includes two components. They themselves are airports them self and air companies. Each sector has its own goals and business politics, but they are connected. Grow of demand on air transport has big influence on the airports and air companies. ICAO and ACI made the forecast for 2010-2017. This forecast asserts that the markets of passengers will growth by 4% -4.5% per year. The Airbus Corporation gives the forecast by 5%-5.3% level. The factors which influence the passengers grow could be enumerated: population concentration, society incomes growth and the state of industry. Also the same situation is with the airports. According to ACI data in 2006 4.4 millions of passengers were served by airports (Central Statistical Bureau of Latvia 2007). It is higher by 4.8% comparing with previous the year. Also the number of the processed cargo is 85.6 millions tons.

One of the main principal differences from the other transport is that some part of the luggage is travelling separately from passengers and presents another material flow. And at the same time each item of the luggage requires registration, security control and delivery to airplane. It leads to the problem of the luggage serving process organization and control. Also the same process must be executed, when airplane arrives to the destination point.

Since Latvia entered the EU in 2004 the international air companies and Latvian national air company AirBaltic got new opportunities in business development. The huge number of air companies and routes lead to the tariffs decreasing, that also leads to the growing of passengers' number. In 2008 the number of passengers reached the mark of 2 millions. According to IATA forecast growth of passengers until 2011 year will be on the level of 12% (the highest in the world). This leads to the problem of the luggage processing in airports.

The main goal of this paper is to describe the experience of using simulation as a tool of the analysis baggage handling system (BHS) in the airport of Riga (Latvia).

MODELLING OBJECT DESCRIPTION AND PROBLEM FORMULATION

There are 4 airports in Latvia: International Riga airport, airport Liepaja, airport Valmiera and airport Daugavpils. In this paper only the baggage handling system of international Riga airport will be discussed. So the BHS could be described as follows. There are 31 check-ins, which are connected with two parallel conveyers. The staff register baggage and put it on the conveyer's belt. Conveyer's belt delivers the luggage to the security zone, where it is checked using x-ray on the restricted items. During this check the security officer takes the decision: if the luggage needs to be checked more strictly or not. If the decision is negative (no additional check is required) the luggage goes to the 1st flow to the equipment area, where the luggage is sorted and loaded to different flights. If decision of the security officer is positive, the luggage

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) should take additional security control using x-ray and it is required the inspection of the officer. If everything is in order, the luggage will be sent to the 1st flow. The scheme and used conceptual model of BHS of Riga is presented in figure 1 and figure 2 accordingly. That is why it is necessary to estimate the effect of passengers' number growth on BHS. For this purpose a simulation approach was chosen. According to (Savrasovs 2008) we can simulate systems on 3 levels: microscopic, mesoscopic and macroscopic.



Figures 1: Scheme of BHS in Riga Airport

The check-in and equipment areas can be called the main problem zones in airport. On the screen of the passengers' number growth these places could become a bottleneck of the whole system.

For this work there was used the discrete-event approach which belongs to the microscopic simulation.



Figures 2: Conceptual Model of the System

The reasons of using the exactly discrete-event approach could be described as follows:

- graphical representation of model must be presented for validation and visualization;
- static and dynamic output must be acquired from the model;
- event-based characteristics of real system

CONCEPTUAL MODEL DESCRIPTION

Before creating the model, the conceptual model should be implemented to ease of understanding of the simulation object. Because the simulations object is very complex some simplifications were done. These simplifications could be easily explained using the conceptual model described in figure 2.

As could be seen in the figure, only 7 check-ins will be modelled. Such decision is connected with the other decision to model only the peak-hours in the airport. For Riga airport those hours are from 17:00 until 20:00.

Mostly these hours are used by the AirBaltic company. That is why only check-ins, which serve the AirBaltic flights are taken into account in the model. The luggage service process was left as described above. The key point of this process could be described in details.

In general the arrival process of entities (passengers) is presented as the poison flow with one parameter intensity. The problem is to determine this parameter, because there were no surveys done in the airport estimating process of passengers entering. But the intensity could be estimated doing the documentation survey. The flights between 17:00-20:00 are mainly the same every day. And the numbers of flights are 14 in this time period. The mean number of passengers for each flight was calculated using the airport documentation. The start of registration is at 120 minutes before the airplane departure. The registration for flight is limited to 100 minutes. So we have got the interval of time of 100 minutes and we have got number of passengers, who came during this time to the registration. Using experts it was determined that the peak of passengers goes between 40-60 minutes before the end of registration. To share the number of passengers at this time period we have used the binomial distribution and Bernoulli formula. The interval of 100 minutes was divided into 10 subintervals and for each interval the probability of passengers appearance was calculated.

$$p_k = C_n^k \times p^k \times q^{n-k}$$

, where n=9, $k = \{0..n\}, p=0.5, q=1-p$

Such procedure was done for each flight. The probabilities were calculated and multiplied by the number of passengers for one concrete flight.



Figures 3: Intensity of Passengers' Arrival Dynamics

The procedure was done for each flight. Data were aggregated for the whole modelling time and the intensity for each subinterval was calculated as could be seen in figure 3

Passengers choose the check-in based on the minimal queue length rule. During the process of registration the passengers must leave their luggage. To define the number of the baggage per person, empirical data were used. The maximal number of luggage per person is 5 items, the minimal is 0. The probabilities are presented in table 1.

Table 1: Probability of Luggage Count

Items count	0	1	2	3	4	5
Pi	0,15	0,65	0,15	0,03	0,01	0,01

The process of registration in general, has fixed the time and depends only on amount of luggage and could be calculated using function below.

$$f(x) = \begin{cases} 30 + x \cdot 15, x \le 5\\ 105, x > 5 \end{cases}$$

where *x* is the amount of baggage items.

So to calculate the time which check-in staff will use to serve the client we are using the constant 30 seconds to register person plus 15 seconds for each luggage item. This time was estimated directly from the check-in staff work observation.

After registering the luggage is put to the conveyer and it starts moving with the constant speed of 0.2 meters per second. The length of the conveyer parts is shown in figure 4.



Figures 4: Conveyer Length

Also here should be mentioned that the probability of the positive decision (needs additional checking of luggage on x-ray point 2) on x-ray point 1 is 0.1. The time of the additional check is distributed by the exponential law with the mean 4. The probability that baggage will be restricted for delivery to the airplane is 0.03. There are two persons in the equipment area who serve luggage sequentially, wasting on each luggage item the time distributed by the exponential law with the mean=13 seconds. Then a luggage car is filled with 30 items of luggage it is send to airplane.

MODEL DEVELOPMENT

As the tool of the model constructing there was used the simulation software ExtendSim from ImagineThat Inc. The reasons of selecting exactly this software can be enumerated:

- Modern simulation system, which has the discrete-event simulation module
- Opportunity of creating 2D and 3D graphical representation of the developed model
- Embedded programming language, which gives more flexibility in logics
- Number of blocks in the discrete-event library which could be used directly
- No limitations on the number of objects used during model development
- Wide number of different random number generators, which can generate the uncorrelated random sequences
- Manager of runs, which does simplification of data collection during runs

Also there could be mentioned that the ExtendSim is widely used in the simulation community for research and analysis. This could be seen from the analysis of the publication at the Winter Simulation conference. The examples of using the ExtendSim for simulation in different application areas could be found in (Damiron and Nastasi 2008; Kopytov et al. 2008; Weiss 2008). In general, the model was developed using the following ExtendSim libraries: discreteevent, item, utilities, value and animation 2D-3D. The item, utilities, value and animation libraries were used as helping libraries for the data collection random numbers generation and visualization. Using discreteevent library objects such as generator, queue, activity, conveyer, combine base model was created according to the conceptual model. The numerical characteristics of the developed model could be mentioned:

- 117 ExtendSim blocks
- 300 connectors
- 2 submodels
- 20 labels
- 29 additional blocks for 3D animation implementation
- 7 blocks for statistics collection

The developed model is presented in figure 5. The presented figure shows that for implementing checkin there was used the sub-model, organized as hierarchical-block. Such approach simplifies the process of using similar parts of model. Also on the base of the implemented model the 3D animation was developed for the visualization and validation purpose. It was done by means of the animation 2D-3D library of the ExtendSim. The base model was completed with special objects.



Figures 5: Model Developed with the ExtendSim

The 3D representation of the model could be seen in figure 6. Using developed 3D animation the base model was validated by means of the experts' approach. Having used animation, the experts concluded that the developed model is valid. The further animation demonstrated different scenarios during the experimental part of work.

EXPERIMENTS PLANNING AND REALISATION

The developed base model was further used for the experiments. There were developed 3 possible scenarios which were played on the model. The description of scenarios could be found in table 2.



Figures 6: 3D animation of the Developed Model

During the experiments the realisation of the structural changes was done in the model. 50 runs per experiments were executed using ExtendSim runs manager. For data collection there were used the blocks from the library value and blocks statistics. During experiments the following characteristics were estimated:

- Utilization of staff in check-in, additional security check and equipment area
- Passengers' queue characteristics (average, maximal)
- Baggage queue characteristics (average, maximal) for the additional security check and equipment area

Table 2: Scenarios Description

Nr.	Description
	• Passengers' flow increased by 15%
1	(forecast until 2010)
	• Number of check-ins is 7
	• Passengers' flow for 2010 (15% growth)
	• 10 check-ins
2	• New staff on 6 check-ins (passengers'
	registration – 50 seconds, 19 seconds per
	luggage item)
	• Passengers' flow for 2010 (15% growth)
2	• 10 check-ins
5	• Passengers' and luggage registration time
	the same as in the base model

The data processing demonstrates that there were some outliered runs in each experiment so these runs were removed as not valid. For the first experiment the number of not valid runs was 3, for the second - 5 and for the third - 6.

RESULTS ANALYSIS

The collected data were analyzed using statistical software (Venables and Smith 2005). The main results could be presented in details visually.

Utilization



Figures 7: Utilization Level on Different BHS Areas

The utilization is used as one of the most important characteristics for determining staff loading level. The figure 7 shows utilization level for 3 different areas of the BHS through 4 earlier described scenarios. The base model is the model, which represents the current situation of BHS. The first cluster of bars deals with the area called "Additional security check", second "Check-In" and the last one "Equipment area". Current mean utilization throw all check-ins is 0.77. This value is relatively in comparison to the normal staff loading level from 0.65 to 0.7. The planned increasing of the number of check-ins in the second scenario does not change the situation, the value of the utilization level becomes worse by 0.79. This points out that the number of check-in plays a big role, but also staff qualification is important and the heads of airport should pay attention to this factor. The last experiment proves that by increasing the number of check-ins we could decrease the utilization, but still decreasing is too low.

All 4 values of utilization for equipment area are high and do not correspond to the implemented normal level of staff loading. Also there should be noted that the variation of utilization level is very low. It means that the passenger flow growing almost does not have influence on the equipment area staff loading. But the reasons of this should be explained.

Also the small variation could be observed in the bars for the additional security check. The values lie in normal range.

Passenger's queue length

This characteristic is used only for check-in, because only check-ins deal with the passengers, all the other work with the luggage. In figure 8 we can see average and maximal characteristics of queue length. The values are calculated through all check-ins.



Figures 8: Average and Maximal Passengers' Queue Length on Check-in

As could be seen the current average passengers' queue length is 35 people and the maximal value is 67. In the first scenario the dramatical changes could be observed. The average length is growing to the value of 57 passengers, but the most important that there is the maximal queue length reached level of 109 passengers. This one is important because the place in the airport near check-ins is limited and as a result the area overloading can happen, which will influence the customers' service level. In the 2^{nd} and 3^{rd} scenarios the value is decreasing and reaches 30 passengers, in average, in the 3^{rd} scenario. Also the maximal value is acceptable.

Baggage queue length



Figures 9: Average and Maximal Baggage Length

The luggage queue can appear in two areas. They are equipment area and additional security check. The figure 9 shows the average and maximal number of items for each zone. Using this result we could conclude that passengers flow growth does not influence match on the presented characteristics. In average there no difference between base model and the 3^{rd} scenario for both areas. But it should be mentioned, that the queue length in the equipment area is very high - 94 items, in average. At the same time the high utilization level for this area (see figure 5) points out that the staff is overloaded. Because of that, this area could be treated as the bottleneck for the system.

CONCLUSIONS

- The model of Riga's BHS was constructed using simulation on the microscopic level, applying the discrete-event simulation approach. As a tool of the model development there was used ExtendSim simulation package. The animation was created for the visualization and validation purposes.
- The input parameters for the model were estimated during document surveys and natural observations of BHS work. Passengers' flow intensity estimation was the main problem during model parameterization. It was successfully solved using binomial distribution and Bernoulli formula.
- 3 different scenarios were implemented for HBS analysis. All of them are based on the hypothesis that during passengers' flow growing, the bottleneck of the system will be in the areas where the manual baggage processing happens.
- Different characteristics were calculated during experimentation. The most important one is the utilizations coefficient for different areas of BHS. The staff loading in the check-ins and equipment area is high and does not fit to the normal defined range. The variation of utilization level is very low. It means that the passengers' flow growing almost does not have influence on equipment area staff loading. This could be explained by the reason that the bottleneck appears between the check-ins and equipment area. Because of the utilization in the check-in is lower than in the equipment area and there is no manual baggage processing between these two areas, we can conclude that the hypothesis that only the staff factor will be the bottleneck in future, could be rejected. The automatic processing should be also taken into account. Speed and conveyers capacity must be increased. At the same time according to the data, the equipment area could be treated as the bottleneck of the system, because of high queue length and high utilization. The additional personnel are required in this area or the baggage sorting must be done automatically.
- The baggage registration procedure must be simplified and self-service possibility should be implemented, because the number of passengers waiting for registration could grow dramatically. Also the increasing number of check-ins could

solve this problem, but staff should have a very good qualification.

• The research must continue to estimate the other scenarios connected with implementing the new conveyers and integrating automatic systems.

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UPGRADING THE TWO-PHASE THERMOHYDRAULIC MODEL FOR THE FULL-SCOPE SIMULATOR OF PAKS NUCLEAR POWER PLANT

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KEYWORDS

Thermohydraulics, nuclear power plant simulation.

ABSTRACT

The upgrade of the full-scope simulator of Paks Nuclear Power Plant (NPP) started in 2008. As a major part of this activity, the original two-phase thermohydraulic module (SMABRE) was replaced by our own development: the two-phase-flow module called RETINA. The validity of the new module was demonstrated by a number of transient calculations comparing the simulation results obtained by the new module with the ones produced by the original module. In the paper we briefly review the replacement procedure with a focus on the differences between old and new thermohydraulic modules. Some simulations results are shown to give some insight on the validation process.

INTRODUCTION

The full-scope training simulator of Paks Nuclear Power Plant has been in service since 1988. In the last two decades practically each element of the simulator has been upgraded, replaced because of the rapid development of the computer techniques making the solution of a great amount of earlier unsolvable problems possible. Moreover, the requirements against the simulator have also been changed. Originally the simulator was used only for training of the operating personnel of the Paks Nuclear Power Plant, but in the last decade it was also utilized as a "test bed" for new systems prior their installation on the real plant.

Changes, however, have not touched two fundamental modules of the simulator viz. the neutron-kinetics and the two-phase thermohydraulics models. Recently, the introduction of new fuel assemblies and consequently the intermediate cores with mixed fuel at the plant gave motivation to take another big step and replace both modules with our codes of own development - in order to simulate better the 3D processes in the core.

Since the simulator plays a crucial role in the life of the power plant such a change needs to be carefully planned, and what is more important, the results obtained by the new modules have to be generally accepted by the operating personnel and the authority. In this paper we focus on the replacement procedure of the two-phase thermohydraulic module of the simulator. The features of the old and new thermohydraulic models are briefly introduced with a focus on differences between them and some simulations results obtained by both modules are presented, too, in order to demonstrate the validity of the new module.

THE REPLACEMENT PROCEDURE

Since the Paks full-scope simulator is a real-time system, each module of the simulator is managed by a scheduler program. It calls various models sequentially taking into account that all modules have to finish their calculation within 0.2 sec. The communication between modules (coupling between models) is clearly defined through the simulator database. Therefore, from computational point of view we just had to follow the basic concepts used for each module of the simulator during the replacement process.

The basic idea was to change the old and new thermohydraulic modules in two steps. In the first step, the nodalization (spatial discretization) of the plant remains the same and we have to demonstrate that utilizing the new module we can obtain practically the same results than we had before using the original module. In the paper we shall focus on this step. In the second step the nodalization of the system will be refined and we have to demonstrate that the simulation results are still reasonable for this new nodalization, too. In these steps, we are going to use the old neutronkinetic module of the simulator, so in a third, final step we are going to replace the neuron-kinetic module of the system, too. Using this strategy, significant changes can happen only in a specific subsystem, which has the same environment than its predecessor. Therefore the identification of the source of a problem encountered during the test procedure is straightforward.

To test the vitality of the new thermohydraulic module a list of transient calculations have been performed and then compared with simulation results obtained by the old code. The list covers a wide variety of physics so it includes such as turbine load rejection, pump and

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turbine trip transients, small- and large-break loss of coolant accidents.

SMABRE AND RETINA: THE PAST AND THE FUTURE

The full-scope real-time simulator of Paks NPP originally had a two-phase flow module called SMABRE. This code was developed to simulate various two-phase flow transients up to the complexity of so-called **SMAII-BRE**ak loss of coolant accidents (LOCA). Nevertheless, as the training simulator in Paks was getting involved more and more into the life of the plant, its scope had to be extended up to the complexity of severe accidents including for instance, the simulation of rapidly evolving large-break LOCAs (Végh et al., 1994; Végh et al., 1995). It turned out that the extension of the code in such directions is not straightforward at all. More and more specific models had to be implemented around the original module making finally the original code somewhat messy.

This fact has given us a strong motivation recently, when the refinement of the nodalization of the system became necessary, to replace the whole code to a new one called RETINA.

RETINA was developed in our institute in 2000. Since it differs very significantly from SMABRE in many respect, it was a quite challenging task to achieve practically the same simulation results with this code than we had before with the use of SMABRE.

Let us briefly summarize the major differences between SMABRE and RETINA. Details are given in (Házi et al., 2001; Miettinen, 1999)

Differences in models and governing equations

Although the same governing equations were implemented in both codes, there are significant differences in the models used to describe interfacial mass, heat and momentum transfer. To be more specific, both models use a five-equation approach (Ishii, 1974; Wallis, 1969), that is two mass and two energy conservation equations are solved for the individual phases (water and steam). The momentum conservation equation is solved for the mixture and it is supplemented by a drift-flux model in order to be able to simulate mechanical non-equilibrium between phases (different gas and liquid velocities) (Zuber and Findlay, 1969).

The original drift-flux model of RETINA was quite different from the one implemented in the code SMABRE. However, our first experiences have shown that the use of the original model leads to very significant differences between the solutions obtained by both codes. This fact forced us to change the drift-flux model of RETINA to a simpler one, close to a model used in SMABRE.

The governing equations need to be supplemented by closure relations, which calculate the interfacial mass and energy transfers in order to close the equation system. There are significantly different closure relations in these codes.

Closure relations are needed for interfacial mass transfer (evaporation and condensation) and interfacial energy transfer (heat transfer between phases). The equation system is also need to be supplemented with models, which take into account heat and momentum transfer between the individual phases and heat structures (walls).

Practically, the same models were implemented in both codes for modeling wall friction (Blasius correlation), but all other models differ somewhat in the codes.

Originally some standard evaporation and condensation models were implemented in SMABRE, but as the times passed by and the simulation scope of SMABRE was extended, more and more specific models had to be introduced into the old code in order to satisfy the new simulation requirements. Furthermore, models used in a certain part of the NPP (e.g. in the pressurizer) were quite different from the ones used in another part (e.g. in the steam generators). This fact made difficult to make any changes to the nodalization of the system, which has became necessary recently.

In RETINA the modeling of evaporation and condensation is in strong relation with interfacial heat transfer models. Basically, correlation for mass transfer between phases were derived rigorously from interfacial heat transfer models making consistent the interfacial mass and energy transfers. In case of SMABRE such relation is not transparent in some of the evaporation and condensation models. In RETINA the interfacial heat transfer models use a simple concept driving back any meta-stable liquid or gas to equilibrium (saturation) with a calculated relaxation time. Using such model, large volumes like the pressurizer or the steam generators of the NPP did not require special treatment. On the other hand, the calculation of the relaxation time proved to be inadequate in some nodes of the nodalization (e.g. at the sprinkler of the pressurizer) and the model had to be tuned somewhat with an additional relaxation parameter.

The implementation of the heat transfer modeling between heat structures and individual phases differs significantly in the codes, although some models used in specific flow regimes have the same origin. As an example we mention Chen's model (Chen, 1966) used to calculate heat transfer in sub-cooled boiling region. Although this model appears in both codes, it is utilized in a quite different manner resulting in some differences in the heat transfer characteristics of the two codes.

The calculation of critical two-phase flow is another example where differences are relevant. This model leads to different break flow characteristics and as a consequence, one might expect that simulation results obtained by the two codes can be significantly different when a loss of coolant accident is simulated.

Differences in the numerical approach

RETINA and SMABRE use significantly different numerical approaches.

Although both codes use similar spatial discretization procedure and staggered grid arrangement for pressure and velocities, their time marching schemes are different. While SMABRE applies a kind of sequential solver, RETINA uses fully implicit time discretization, calculating the Jacobian problem by automatic derivative functions.

The application of a fully implicit solver has some drawbacks. In general, an implicit solver needs some iterations to find the solution of the problem in question; and using large time steps for a very fast transient, one might encounter convergence problems, because of the overestimation of the elements of Jacobian matrix.

Originally, RETINA used automatic step size control to avoid divergence of the solution and the number of iterations used in each time step was controlled by the norm of the corrections used in each iteration. This strategy proved to be inappropriate for a real-time application. Therefore the time step was finally set to 0.2 sec and the number of iteration in each time step was limited to one. As it will be demonstrated, the code is still able to calculate any relevant problem with reasonable accuracy - even using such a strict limitation.

SIMULATION RESULTS

The new thermohydraulic model has been tested by performing 10 reference calculations with SMABRE (Bürger et al., 2008) and repeating these calculations by RETINA. The environment of the codes was the same, namely the full-scope simulator of Paks NPP.

Practically, we had performed a run with SMABRE and than changing the thermohydraulic module, we repeated the calculations using the same initial condition with RETINA. Results obtained by the code were monitored by the Instructors' system of the simulator.

At the beginning of this procedure we had to obtain a steady state with RETINA with a prescribed accuracy (differences had to be less than 2% for each relevant physical variable) using SMABRE results as reference.

In Fig. 1 the results obtained by initiating 1^{st} turbine trip of the NPP are shown. On the left (from 0 to roughly 25 minutes) and on the right (from 25-50minutes) the results of RETINA and SMABRE can be seen, respectively. The plot shows the pressure of the pressurizer, the position of the turbine control valve, the pressure of the steam collectors on the lost and working side, the water level and pressure of the 2^{nd} steam generator.

In this scenario the failure of the turbine control valve causes an immediate turbine trip. Since the steam collectors are connected, therefore the pressure is rapidly increases in both sides, until it reaches the activation pressure of the collector blow-down valve (48 bar). The blow-down suddenly decreases the pressure of the steam generators, which leads to intensive boiling and the swelling of the water level.



Fig. 1 Simulation results obtained by RETINA (left) and SMABRE (right) for turbine trip.

In Fig. 2 the simulation results of tripping three pumps are shown - plotting some relevant quantities, i.e. the reactor power, the water level and pressure of the pressurizer, pressure of the steam collector, and the water levels of the 1^{st} and 2^{nd} steam generator.

The test scenario is as follows: Due to power failure, the primary circulating pumps stop in the 2^{nd} , 4^{th} , and 6^{th} loops. The flow rate decreases in the core and the coolant adsorbes more heat from the fuel increasing the pressure in the primary circuit. Accordingly, the reactor control system reduces the power level by ~40% and as a consequence the pressure falls down again to the nominal value.



Fig. 2 Simulation results obtained by RETINA (left) and SMABRE (right) for the trip of three main pumps.

Finally, in Fig. 3 the results of the calculations obtained by both codes for the opening of the pressurizer's safety valve can be seen. The relevant quantities shown in the figure are the following: pressurizer pressure, flow through the safety valve, level of the pressurizer, pressure above the zone, pressure of the relief tank and the water level in the containment.

In this test the pressurizer safety valve opens and the pressurizer starts to blow-down into the relief tank. The pressure rapidly increases in the relief tank until its rupture plate breaks and the coolant blows-down to the containment.



Fig. 3 Simulation results obtained by RETINA (left) and SMABRE (right) for opening of the pressurizer's safety valve.

As it can be seen, the results of RETINA are practically the same than that of SMABRE for each of these transients. No relevant differences can be observed in the physical parameters, although the codes are quite different considering their models and numerical approaches.

CONCLUSION

Although the change of a physical model in a simulator may seem to be a straightforward task, our experiences show that such a work can bring serious challenges depending on the complexity of the modeling problem. The replacement of the two-phase thermohydraulic module of the real-time full-scope simulator of Paks NPP has been briefly reviewed in this paper.

In spite of the fact that there are significant differences between the implementation of the new and old modules considering their models and numerical methods, the results obtained by the new module are in good agreement with the ones obtained by the old one.

However, it should not be so surprising, since the underlying physics addressed by both codes are the same. Therefore the good agreement is partially due to the facts that the numerical approaches together with the models used in the codes are describing reasonable well the real physics. From another point of view, it is also a result of the control system, which drives both models in the same way as far as their output remains accurate enough.

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MODELLING LAYOUT FOR INTEGRATING SIMULATION, OPTIMIZATION AND VIRTUAL REALITY

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KEYWORDS

Simulation, Genetic Algorithm, Optimization, Layout Engineering

ABSTRACT

The aim of this research is the development of an innovative approach to support company upgrades, reorganization and new facility establishment. This approach is focused on combining layout engineering with the use of simulation and optimization; this combination is very important because allows to reorganize the whole layout and production processes and flows and to measure the results in the virtual world before making real changes. The proposed methodology is applied to a real case study: the reengineering of the production plant layout in an aerospace company moving to a new site.

INTRODUCTION

The Layout analysis is a well know application area for both simulation and optimization; in fact the necessity to consider the interactions among many different variable, often affected by stochastic behaviors, support the use of complex models and the application of simulation methodologies; in this area often the problems are becoming pretty complex in term of size of the problem or type of the components. In these cases the optimization techniques are often dynamically interacting with the simulator in order to proper estimate the performances of the new proposed layout.

In this paper the authors are presenting a methodology derived from these cases that combines different models: simulation models related to production flows, intelligent optimizers based on Genetic Algorithms (GAs) and Virtual Environments for presenting the dynamic nature of the phenomena and their evaluation along the whole production site construction.

In fact in this case the final goal it concentrates not only on optimizing the layout, but much more in obtaining a robust solution that could face the market evolution and that could support the whole factory transitory: from the dismissing of the old one to the completion of the new facility. In this inter reign it is critical to guarantee the production levels by a proper planning and a proper layout organization as well a proper factory movement schedule. The authors developed a solution for considering all these aspects defined as LEXIS (Layout Integrated Solutions) which Excellence & is implemented in C++ while VEGATM is the commercial solution for 3D. Therefore LEXIS project integrates Layout Optimization based on Genetic Algorithms, Modeling & Simulation and Virtual Reality for supporting the development of a new large Production Facility for an Aerospace Industry. In fact Lexis aims to create a model that maximizes the layout of an aerospace production.

This paper provides the description of the model used for constructing the simulator to be integrated with the optimizations paper.

THE PROJECT MOTIVATION

The project motivation is related to the aerospace company reorganization; currently the company includes two main production facility: the first one devoted to planes manufacturing and engine components, and the second one focused on the whole aircraft assembly.

In fact it has established the transfer of the manufacturing plant in a new area; in fact the old facility was developed during WWII and the layout was strongly affected by related considerations. Today market evolution proposes new opportunities for setting up the production site and it was making sense to evaluate alternatives.

The Company production facilities cover 120,000 square meters (1.3million square feet) in the northwest of Italy. Nowadays the company is building a new stateof-the-art facility, designed to implement the latest lean manufacturing technology that substitute one of the existing production site. This lean philosophy will increase production capacity, efficiency and optimize workflow, building this facility in response to the rapid expansion of its business. The new production facility, called in the following figures "site N", will better position the company to successfully meet the challenges of the market. Final aircraft assembly, flight-

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testing and aircraft overhaul operations are located at the corporate headquarters (site 1). The company service center offers full service support to its aircraft and aircraft under Jar 145 certification.

Aircraft and engine components, manufacturing, general engineering, engine maintenance and overhaul are based on production site 2. Operations include a maintenance center and two production areas, one for engines and sheet metal parts, another for major aircraft subassemblies.



Figures 1: Production Flows

The object of this work is to optimize the layout of the production flows and to guarantee the transitory during the change from the old facility to the new one.

The project is divided into different main phases:

- Data Collection and Certification
- Production Flow Definition
- Simulation Development
- Synthetic Environment Integration
- Layout Optimization

Before to activate the modeling research it was requested by the company to evaluate different implementation solutions in order to guarantee the users with the capability to maintain the simulation implementation. Different COTS (Commercial Off-the-Shelves) have been evaluated in term of their technical and functional aspects:

- Layout Optimization Capabilities
- **Graphics Capabilities**
- Compatibility with other Software
- Maintainability & Stability
- Acquisition, Service and Training Procedures

In the proposed case the company is composed by a production machinery set over passing 400 entities; in addition to these elements it becomes necessary to define all the warehouses and the areas for work in progress (WIP); in addition architectural elements, and ancillary entities have to be consider as part of the whole layout.

LEXIS ARCHITECTURE

The proposed architecture expect to integrate three different modules: the simulation model, the Optimizer and the Synthetic environment.

In fact the simulation represent the core to be interrogated by the Optimization system; the authors are currently presenting the simulation model, while the following step will be the integration of the optimizer; this module is based on genetic algorithms considering the number of variables that need to be optimized and the benefit of this approach in using user proposal as seeds for the optimization process.



Figures 2: LEXIS Architecture

CONCEPTUAL MODEL

The proposed methodology is based completing the creation of a simulation model based on OODA (Object Oriented Design and Analysis).

In fact the following objects was defined for representing the elements of the layout problem:

- Layout Object
 - Layout Object (LO) ID Id_{LO}
 - $S_{\rm LO}$ LO Status
 - Orientation α_{LO}
 - DxLO, DyLO, DZLO Delta Position from Department Reference Point i)
 - Fnx_{LO} , Fny_{LO} , Fnz_{LO} Foundation Size (X,Y,Z)

LO Code

- FnmLO
- Foundation Mass $\text{Fn}S_{\text{LO}}$ Foundation Surface
- LO Size (X,Y,Z) LxLO, LyLO, LZLO
- La_{LO} LO Area
- PDI/ACILOProduction Department Id
- and Activity Cost ID i) LO Description
- DescriptionLO
- CodeLO
- Constructor_{LO} LO Constructor LO Model
- $Model_{LO}$ LO Type
- Type_{LO}
- DepartmentLO LO Department

•	SmokeLO	Smoke Evacuation Requirements
•	Pr _{LO}	Productivity
•	Mob _{LO}	Mobility
•	NoiseLO	Noise Generation Level
•	SensLO	Sensibility Grade respect Noise
•	SOLO	Operating Status
•	Disp _{LO} devices)	Availability starting date (new
•	LineLO	Production Line
•	TimeLO	Expected Time required for

moving from old to new facility

Service Box

•	id _{SB}	Service Box(SB) Code
•	lo _{SB}	Associated Layout Object
•	dx _{SB} ,dy _{SB} ,dz _{SB}	Distances from LO Reference Point
•	lx _{SB} ,ly _{SB} ,lz _{SB}	SB Size
•	ß	SB Orientation

Flows

•	id _f	Flow Code
•	Type _f	Flow Type
•	S_{f}	Description
•	From_Where _f	SB Origin
•	To_Where _f SB Destin	ation
•	MainProductID _f	Main Product ID
•	Items/MainProduct _f	Production Ratio
•	ItemID _f	Item ID
•	Code _f	Item Code
•	T _{f1}	Set Up Time
•	T _{f2}	Unit Production Time
•	LT _f	Production Lot

Products

•	id _p	Final Product ID		
•	$\mathbf{Q}_{\mathbf{p}}$	Planned Quantity		
•	Coden	Final Product Code		

Items

idi	Item ID
Si	Item Description
Sx _i , Sx _i , Sx _i ,	Item Size (X,Y,Z)
Ni	Number in Packaging Unit
MM_i	Movement Mode
Code:	Item Code

Corridor

•	id _c	Corridor ID
•	Type _c	Corridor Type
•	Description _c	Corridor Description
•	From_Where _c	Starting Node
•	To_Where _c	Ending Node
•	Size _c	Corridor Size

Corridor Node

•	id _{cn}	Corridor N
•	Type _{cn}	Corridor N
•	Description _{cn}	Corridor N
•	X _{cn} , Y _{cn} , Z _{cn}	Corridor N

- Handling Device
 - $\mathrm{Id}_{\mathrm{hd}}$
 - Type_{hd}
 - Description_{hd}
 - Caphd
 - Coshd
- ode ID ode Type ode Description lode Location

Handling Device ID Handling Device Type Handling Device Description Handling Device Capability Handling Device Cost

Speed _{hd}	Handling Device Speed
N _{hd}	Handling Device Numb

- Handling Device Number
- **Production Department**
 - ID Dp LO Department
 - Department Description S_{Dp}
 - Department Orientation $Dp\eta_{Dp}$
 - Dpx Dp,Dpy Dp,Dpz Dp Department Location (X,Y,Z)

Layout Objects represent both machinery components, architecture elements, offices, warehouses, testing areas etc.; each Layout Object (LO) can be associated with one or more Service Boxes; each Service Box (SB) is in charge of being the connecting point for the Flows and can serve as input, output or input/output point for a machinery or a warehouse; the system is defined in 3D even if most of the optimization is expected to work on 2D. The basic structure of the LO and SB in term of space occupation is proposed in the following picture.



Figures 3: LO and SB Structure

The Flows represent a logical connection between two Service Boxes; Flows can be associated with different Items; Items usually represent raw materials, components, intermediate products, finished goods, however it is possible to use Items for defining flows of resources, people, data. The Handling Devices are used in order to define the effort required to transport the related items over a Flow based on their capabilities (i.e. unit time, capability, unit cost), while the Item quantities are attributed to each Flow in relation to the final product quantities, by this approach all the quantities and costs are easily updated based on production mix expectations.

A general scheme of the Flows in the Layout is proposed for an example involving two different final products (A & B) is provided in the following picture.



Figures 4: Flows Scheme

DATA COLLECTION METHODOLOGY

In order to proceed in the analysis it is critical to acquire all the information and data required by the model; in this phase it is critical to collect data, to acquire knowledge and to proceed in information certification.

In relation to the production machinery components it is important to acquire: technical details (i.e. foundations, productivity, size, service required), technical drawing (layout element shape) and process definition (bordering areas for WIP). These things allow to define the machines into the simulator, and it can be possible to evaluate the volumes for the related buffers and to define the optimum layout to facilitate the loading and unloading of materials. It was defined as an active LO each element that is hosting a task or production process, while as passive elements it was defined the entities representing architecture component, infrastructures or ancillary objects.

Scenario definition

A critical step in simulation projects it is the scenario definition; in the layout optimization it is necessary to consider different components defining the scenario to assess the effects that different hypotheses can generate. In particular it is critical to define alternative market evolution scenarios; in fact in the near future it is usual to expect changes over time in demand of the different finished products; the layout obviously need to be robust to face the changes in the flows in term of volumes.

Production elements

As anticipated the proposed methodology was applied to a real Case Study; in this case the data collection required strong liaisons with company experts of the different division (industrial engineering, processes, production, maintenance, etc.); in this case the solution was developed also in order to support the production process re-engineering based on the opportunity to set up the new production facility.

During the data collection it was evident the missing interconnection among the data in fact the available information resulting in this case was including, as usually:

- Bill of Material (BOM)
- Machine Parameters & Drawings
- Production Process Definition & Task List

However the very important information related to the processes not directly connected with machines was not structured: i.e. the testing activities and the necessary devices and equipment as well as the acceptance areas and checking procedures.

In addition the production in this reality involved different general products: engines and aircraft and all the data structures was divided and with different format.

So it was necessary to combine the Production Processes with the BOM in order to define the sequential procedures for production of the finished goods as well as the structure of the initial, intermediate and final warehouses.

However the production processes include tasks to be carried out in the production facility in examination, outsourcing as well as other production plant activities; so it is necessary to extract the items related to the layout based on task list definition; obviously the model requires to be flexible in order to compare solution where tasks are moved inside the layout or outside (by outsourcing for example).

Bill of materials

The Decomposition of the main products in term of elements is a fundamental element for extracting the items to be attributed to the production flows. The BOM is usually structured as a tree, with the final product at the top, and then the different levels exploding down it in components, sub-components, etc. In the proposed case study the BOM was characterized by 14 different levels.

Task & Machinery Lists

For each element required by the Task List it was defined a set of two different Identifiers: Production

Department Id (PDI) and Activity Cost ID (ACI); by this approach it is possible to support planning and to estimate the added value of each operation in the production process. As input data it was used the database issued by the maintenance department including description of the machines, this list was extended including all the areas required by the tasks and processes based on review of production process definition and task list with subject matter experts.

In fact it is critical to complete as soon as possible the full list of all required active LOs in the plant; obviously the support from company experts is fundamental.

However the Machine database, developed by maintenance department, was mostly driven by the necessity to support the factory movement in the new facility; so it was structured based on new machine acquisitions and existing element listing for the movement; it is evident however that by this approach, the machine tables could result inconsistent respect the PDI/ACI list. In fact it is interesting to outline the presence of "exceptions" that have to be "normalized" to be included in the model; in fact there are machines that are defined in term of PDI and ACI, but are still missing a single code, being in fact an entity resulting from the merging of many different elements and small machines; at the same time it is possible to have areas that was identified as an element in the task lists but that still miss the Id code for the factory movement

The following picture propose an example of the current situation and the relative definition of elements respect its production department; in order to combine the two data set in a single consistent element it was necessary to avoid duplications and to identify connection; the authors was working with Subject Matter Experts (SME) in order to define proper level of detail for modeling the active elements representing Layout Objects



As result of this phase it was possible to add to the LOs to be moved in the new facility or to be acquired, also the elements that aren't "real machines", but that represent critical Layout Objects: for instance testing areas and working banks.

By this approach the list of entities was representing all the "active" Layout Objects.

The authors decided to collect also four pictures for each machine, one of each side; the aim of this activity was to insert them on the cubicles that was expected to be used in the 3D representation of the Layout Objects.



Figures 5: Collecting images for 3D representation

Current Layout

Using the company CAD files, it was possible to measured the current position of each machine in relative coordinates respect its production department, as well as the position and size of each department; obviously it was necessary to extract also all the positions for warehouses and buffers in each department.

These data was collected in order to being able to estimate current layout effectiveness as reference value for comparison with the new plant solution; in addition the relative coordinates of LOs could represent a proposal for the new plant layout with a simple relocation of the departments; this solution is obviously a very limited optimization, however represent an interesting reference value for comparing new solutions and new production planning strategies.

Architectural Elements

Therefore it is necessary to collect the information about the infrastructure of the new facility such as its size, narrowness of the wall, material structure, position of the columns, position of the toilets, the offices, foundations, special plants and the emergency exits.

So the next step was to complete the LOs by extracting all the architectural elements from the future factory blueprints; these elements was including both fixed (i.e. pillars, underground escape routes) and mobile (i.e. offices or element not yet finalized in term of position and characterized by degree of freedoms in locations) items; the related characteristics was introduced in the LO definition.

EXPERIMENTAL ANALYSIS

As anticipated the first phase was to apply the proposed model in order to reproduce the actual layout of the production under reorganization and the related flows of the material and information.

Currently the authors are working in carrying out the experimental analysis on the current and new layout. The verification and validation of the model was strongly based on joint review with SME and final users, as well as statistical analysis of the simulator results.

In the following picture is presented a synthesis of the simulator GUI (Graphic User Interface) presenting overall flows and LO for a case study.



Figures 6: Flows and GUI

CONCLUSION

The paper proposes an approach for modeling industrial facility in order to face layout optimization by an integrated approach; the proposed methodology, LEXIS, demonstrates it consistence with Lean Simulation approach and was successfully applied to the real case study of a large production facility in aerospace industries.

The authors are currently finalizing the optimizer integration in the LEXIS architecture and in completing the simulator fine tuning.

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SYMBOL NAMING RULES FOR PLANT MODEL GENERATION IN THE PLC SIMULATION

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KEYWORDS

Programmable Logic Controller (PLC), PLC Symbol, Simulation, Virtual Factory

ABSTRACT

Presented in the paper is the PLC symbol naming rules in order to simulate the virtual factory which is operated by the PLC control logic. In the PLC simulation, the corresponding model, normally called as the plant model, to the PLC receives the PLC output signal, operates virtual devices, and sends the changed PLC input signal which is updated by the virtual device movements. Therefore the plant model is necessary to verify PLC code and to simulate the virtual factory. Normally, the plant model construction takes much time and effort, requires in-depth knowledge about the simulation and PLC code, and even it might has modelling errors. To prevent the modelling error and to save the time and effort for the I/O model construction, this paper proposes the naming rules of PLC symbol to extract the necessary information. The simple example cell is applied to test the proposed approach.

INTRODUCTION

To survive and prosper in the modern manufacturing era, a manufacturing company should be capable of adapting reduced life cycle of products in a continuously changing market place. Simulation is a useful tool for manufacturers to adapt this kind of rapidly changing market to design and analyze complex systems that are difficult to model analytically or mathematically. (Choi and Kim 2000) Manufacturers who are using simulation technology can reduce the time to reach the stable condition of automated manufacturing system by utilizing statistics, finding bottlenecks and pointing out scheduling errors etc. The discrete event system simulation makes possible to extract these kinds of simulation results. (Klingstam and Gullander 1999; Al-Ahmari and Ridgway 1999) ARENA and AUTOMOD is widely used for discrete event system simulation software.

Other than the discrete event system simulation, there is another very important concept which has to be considered in today's simulation environment. With the huge improvement of computing power, many user want to create much more realistic simulation model,

which can forecast not only the production capability of the system but also the logical verification, physical validity, and the efficiency of co-working machines. The demand results in the concept of virtual factory (VF), which can be described as a model executing manufacturing processes in computers just like the real world. (Onosato and Iwata 1993; Onosato et al. 1995; Lin et al. 1999) Because the delay in construction of the automated production line and the line stop during the automated mass production system cause the large loss of revenue for the manufacturing company, the VF simulation technologies for process validation prior to the real implementation are becoming more important in many manufacturing areas. Especially, not only showing the movement of the automated virtual devices, but also the running with real control logic. Simulation running with the real control logic is getting important to verify the production system. Control program verification and validation is a rising topic among the current control engineers.

After the successful programming of a Programmable Logic Controller (PLC) code, in conventional control logic verification, checking the correctness of the program is a mandatory job in a shop floor control system. The accuracy of the control logic plays a vital role in the automated manufacturing line for the proper functioning of the production process. (Lucas and Timbury 2003) Normally the PLC verification work has been done manually. This process typically starts with writing the PLC program as per the IEC 61131-3 standard. (IEC, 2003) In next step, the program is downloaded to the PLC, then the input value is provided or changed by the user to check the logical flow of the program. Finally, the PLC program can be simulated by giving the Boolean inputs manually. Although it is easy to check the short and small scale of control code, the checking of a large and more complex program is almost impossible as it is a time-consuming and error-prone process. In addition, it is very difficult to decompose complex PLC code manually and to verify all possible dynamic properties. (Younis and Frey 2003)

To solve the aforementioned difficulties of simulation running with PLC code, the counterpart model which is corresponding to the PLC signal is necessary. Generally, it is called the Plant model. The Plant model receives the PLC output signal and operates the virtual devices in the 3D space. According to the movement of virtual

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device, the renewed signals such as the sensor detection of virtual device movement is sent to the PLC as a PLC input.

There have been several approaches for the Plant model. A simple real-time I/O simulator was proposed to test the PLC program, in which the benefits of an objectoriented simulation approach to perform control program testing quickly was introduced. (David 1998) However no concrete methodology and result were presented. A virtual factory consisting of a 3D graphic model and behavior model was combined with an actual factory to verify the ladder program in the PLC. (Hibnio et. Al. 2006) Park et al. proposed the I/O model as a Plant model which can interchange the signals with PLC. (Park et. al. 2006)

In I/O model approach, the virtual devices are represented with the device states. The state changes are caused by the PLC output signal. Once a state is changed by the PLC signal, the corresponding signals derived by the state change is transfered to the PLC as an input. Even though the I/O model is easy to understand and to construct, constructing the I/O model is time consuming work. Especially the field workers are not willing to construct another work (model), namely I/O model, to verify the PLC code. In addition, if the process scale is as large as the line level, there are not only the huge effort to construct the I/O model, but also some possibility of I/O model error in itself. To overcome the mentioned problems, the I/O model is supposed to be generated automatically. The input factors for constructing the I/O model are PLC code and PLC symbols. Originally, the I/O model is constructed by analyzing the PLC code and PLC symbols which is named with no dominant rule depending to the programmer's propensity are used in the code. Consequently, this paper proposes the naming principle of PLC symbols to construct the I/O model automatically. The presented PLC symbol naming principle permits to contain the necessary information to the symbol to construct the I/O model automatically. With the proposed methodoloty, the PLC simulation is ready to do just by importing the symbol list to the simulator.

PLC SIMULATION

The Programmable Logic Controller (PLC) is a dedicated industrial computer used to control automated processes in manufacturing. (Parr 1999) PLC is designed for multiple inputs and outputs arrangements and it detects process state data through the sensing devices such as limit sensors, proximity sensors, or from the signals of the robots. It executes Boolean logic according to updated input memory and triggers the next command to the actuator such as motor, solenoid valve or command signal for the robots etc. PLC code can be represented in different types of languages. IEC published IEC 61131-3 to standardize PLC languages including Ladder diagram, Sequential Function Chart,

Structured Text and Function Block Diagram. (Maslar 1996)

"RHGate_ L5_LS_CRP_ CHK2"	"LHGate_ L5_LS_CRP_ CHK1"	"LHGate_ L5_LS_CRP_ CHK2"	"RH_M_LD5_ CR_PART_ ON" ()	
itle:				
"RHGate_ L5_LS_CRP_ CHK2" 	"LHGate_ L5_LS_CRP_ CHK1"	"LHGate_ L5_LS_CRP_ CHK2" 	"RH_M_LD5_ CR_PART_ NONE"	
itle:				
"RHGate_ L5_LS_ PART_CHK2" "RH_M_ RBT7_2nd_ cowp."	"5000times	"RH_M_LD5_ PART_ON" (S)		
	LS_LS_CRP_ CHC2" "RHGate_ LS_LS_CRP_ CHC2" It le: "RHGate_ LS_LS_CRP_ CHC2" It le: "RHGate_ LS_LS_ PART_CHC2" H "RHGate_ LS_LS_ PART_CHC2"	LS_LS_CRP_ LS_LS_CRP_ CHC2" CHC1" CHC2" CHC1" CHC2" CHC1" CHC2" CHC1" itle: "RHGate_ LS_LS_CRP_ LS_LS_CRP_ CHC2" CHC1" itle: "RHGate_ LS_LS_ PART_CHC2" H "RHGate_ LS_LS_ PART_CHC2" H "RHGate_ LS_LS_ PART_CHC2" H	LS_LS_CRP_ LS_LS_CRP_ CH(2" CH(LS_LS_CRP_ LS_LS_CRP_ CH(2" ON" CH(2" OH(" CH(2" ON" CH(2" OH(" CH(2" OH" OH(" CH(2" OH" It le: "PHGate_ "LHGate_ "HGate_ "RH_M_LD5_ LS_LS_CRP_ LS_LS_CRP_ LS_LS_CRP_ CH(2" NONE" CH(2" CH(2" CH(2" OH(" OH(" OH(" OH(" OH(" OH(" OH(" OH(

Figure 1: PLC Code Example in the form of Ladder diagram

A PLC can be considered as a system having input and output in essence. To run a PLC, a counterpart system which is called Plant Model is required to interact with the input and output of the PLC. The behaviour of the Plant model should be similar to that of the actual system to achieve correct PLC verification. Thus, the procedures start with the virtual modelling of the actual manufacturing system. Simulation is conducted to check the behaviour of the entire system. If desired behaviours are not observed or undesired behaviours are observed in the simulation result, then the code errors can be corrected such as robot conflict, non detection of emergency condition and over run problem. The verification architecture of the PLC simulation is shown in Figure 2.



PLC Program Figure 2: PLC Simulation architecture

I/O MODEL AS A PLANT MODEL

Manufacturing devices consisting the process line can be divided into three categories. The first are intelligent devices (such as a transporter, handling robot and welding robot), the second are simple actuators (JIG, servo motor) and the third are sensing systems (proximity sensor, light sensor). Because the PLC controls various counterpart devices, virtual process is also needed to model the each resource to correspond to the PLC. As a counterpart modeling (Plant model) technique, this paper employs the I/O model. (Park et. al. 2006) The I/O model is to describe the devices of virtual process line using a state-based object model. The principles of the I/O model involve device modeling with the PLC point of view, which is focused on the control signals and decomposition of the entire system according to their functional role as many as possible. The user can imitate the target system using a finite set of an I/O model, including operations, states and events. And the I/O model receives the PLC output signals and sends the corresponding signals as the PLC inputs. The specified I/O model consists of eight denotations:

 $M = \langle I, O, S, \delta_{int}, \delta_{ext}, \lambda_{enter}, \lambda_{leave}, \lambda_{disable} \rangle$ I : input set O: output set S: state set $\delta_{int} : internal transition function$ $\delta_{ext} : external transition function$ $\lambda_{enter} : entering output function$ $\lambda_{leave} : leaving output function$ $\lambda_{disable} : disable function$

In the components of an I/O model, a device is partitioned into a set of states, inputs and outputs. The behavior of a device is defined by five function-sets: external/internal transitions, entering/leaving output functions and a disable function. The behavior of the system is controlled by the PLC, which sends signals to I/O model. An external transition function changes its state when it receives external input from the PLC: $\delta_{ext}(A, I \mid \Delta t) = B$ represents "If the current state is A and the model receives external input I, then the state will change to B during Δt ". An internal transition function describes an automatic transition during a predefined time: $\delta_{int}(B \mid \Delta t) = C$ represents "If the current state is B, the state will change to C during Δt time. The entering output function generates an outgoing message to the PLC when the model enters a state: $\lambda_{enter}(B) = O_1$ indicates "If the model enters State B, then the function emits a O_1 signal to the external controller (PLC). The leaving output function generates an outgoing message to the PLC when the model leaves from a state: $\lambda_{leave}(B) = O_2$ indicates "If the model leaves State B, then the function emits a O_2 signal to the external controller (PLC). The disable function sets a specific I/O model to disabled mode when the model enters a state: $\lambda_{disable}(B) = M_1$ indicates "If the model enters State B, then the model M_1 is disabled; if the model leaves State B, than the model M_1 is enabled." This method is useful for the modeling of automated process line from the point of view of the controller. The graphical notation of an I/O model is shown in Figure 3.



Figure 3: I/O model as a methodology of Plant model

PLC SYMBOL RULE FOR THE I/O MODEL AUTO GENERATION

Even though the IEC 61131-3 standardized the PLC in many aspects, (Parr 1999) the PLC symbol name structure is not defined. In the real field, there is no rule for the symbol name. It varies from the PLC programmer's naming habit and from the different PLC vendor because of hardware characteristics. As a result, only the PLC programmer can recognize the exact usage of a symbol from the name. Here the necessity of the standardization of symbol name is found to extract the meaningful information from the symbol name.

Generally, the symbol name can be partitioned by under bar ('_'). Despite of this is a general truth; there is no detail rule which indicates the process information. This paper proposes the naming principle to generate the I/O model automatically.

The I/O model contains each device's state and related signals, which can change the state or device movement and can report the device's state. Therefore, symbol name need to have the device information, especially the device hierarchy or the involving higher level process information for the larger line. In addition to the device information, the states are needed to be defined in the symbol name to generate the states for each device. In case of Operation, this signal is the PLC output signal which changes the device states. By putting the next state name to the operation name, we can extract the state and operation name at the same time. From the state change, the event will report the state change to the PLC. Unlike the operation is the PLC output signal, the event signal is the input for the PLC. Therefore we can give the similar name pattern to the signal just by distinguishing if the one is input or output signal. Proposed signal structure is shown in Figure 4.

SYMBOL structure

Level 1	Level 2	Level 3	_[Level 4	Level 5	
Level	Contents			example		
Level 1	Line name			BB(body build)		
Level 2	Process number			S301(station 301)		
Level 3	Device name			RBT3(robot3)		
Level 4	Input or Output			l or O		
Level 5	Task			WELD(welding)		

Figure 4: Proposed PLC Symbol structure

In the procedure of the I/O model auto construction, the information from level 1 to level 3 is referenced to recognize the device, extract all the related symbols for a selected device, and to create device hierarchy in terms of whole process line.

Once the related symbols for one device are extracted, next step is to create the device states. Among the PLC output symbols whose 4th name field is 'O' is used to create the states. The 5th name field information of operations symbol indicates the terminal state, namely this operation is a triggering symbol to that terminal state.

The remained work is to assign the PLC input, namely event symbol in the I/O model, to the each state. The Event symbols are the symbol which senses the state changes and report to the PLC as a PLC input. The Event symbol is recognized by the 4th name field of symbol. If 4th name is showing the 'I', this means that current symbol is PLC input symbol, which detects the state in 5th level name field and transfer the signal to the PLC. While the operation symbol indicates the next state which will be reached by the this operation symbol, the event symbol show the current detected state. With this method, the symbols will be referenced to generate the I/O model automatically. Detail procedure and example is shown in next chapter.

EXAMPLE CELL AND IMPLEMENTATION

In this chapter, we will observe a small work cell example. Figure 5 shows the small cell example. At first, an entity will be generated. Then this will lay on the AGV machine in P1, then the AGV senses this raw part and moves to the P2 for machining. When the machine detects the part arrival by the AGV in P2 position, the machine starts to operate. We can consider two devices in this example cell for the I/O model, the AGV and the Machine .



Figure 5: Example Cell

The AGV model can have two states. One state is when the AGV is in P1 position and another is when the AGV is in P2. Therefore, it has two input signals that sense the each position, and two operation signals that command to move. With the proposed symbol naming rule, we can give the signals for inputs as 'EXCELL_MB_AGV_I_P1',

'EXCELL MB AGV I P2'. Here, it is assumed that process name is MB (Main Buck). Similarly, we can make the operation signals. The first one is 'EXCELL MB AGV O P2' that command to move to the P2 position from the P1 position. And the second is 'EXCELL MB AGV O P1' that commands to move to the P1 position from the P2 position. In case of Machine device, the states can be defined into two. The first one is the Idle when the Machine is not operating or waiting for the next raw part. The second is the Run when the machine is running. Likewise the AGV symbols, we can create the symbols of the Machine. The event signals can be'EXCELL_MB_MC_I_IDLE1', 'EXCELL_MB_MC_ operation I_RUN2', and the can be 'EXCELL_MB_MC_O_IDLE1',

'EXCELL_MB_MC__RUN2' respectively. The number in the last digit of the level 5 means the state sequence. The machine is on IDLE state at first and it changes its state to the RUN.

	A	В	C	D	E	F
1	Class	Identifier	MIT-Addr.	IEC-Addr.	Туре	Initial
2	VAR_GLOBAL	EXLINE_MB_AGV_I_P1	X0001	%IX0001	BOOL	FALSE
3	VAR_GLOBAL	EXLINE_MB_AGV_I_P2	X0002	%IX0002	BOOL	FALSE
4	VAR_GLOBAL	EXLINE_MB_AGV_O_P2	Y0001	%QX0001	BOOL	FALSE
5	VAR_GLOBAL	EXLINE_MB_AGV_O_P1	Y0002	%QX0002	BOOL	FALSE
6	VAR_GLOBAL	EXLINE_MB_MC_I_IDLE1	X0003	%IX0003	BOOL	FALSE
7	VAR_GLOBAL	EXLINE_MB_MC_I_RUN2	X0004	%IX0004	BOOL	FALSE
8	VAR_GLOBAL	EXLINE_MB_MC_O_IDLE1	Y0003	%QX0003	BOOL	FALSE
9	VAR_GLOBAL	EXLINE_MB_MC_O_RUN2	Y0004	%QX0004	BOOL	FALSE

Figure 6: Symbol list according to the proposed rule

With the example cell, the PLC symbol list is presented in Figure 6. This list is formatted for GX IEC developer version 7.0 produced by Mitsubishi Electric Corporation. The above Excel file format can be acquired by exporting the symbol table from the GX IEC developer, in which the symbols are declared and the PLC code is programmed as well. Once the symbol list is decided, it will be inputted to the simulator which is comprised of the I/O model and the virtual graphic factory. Figure 7 shows the generated I/O models in a simulator after importing the PLC symbols. As we can see, the device I/O models are suspended in 'ExLine' project tree. And two I/O models are generated.



Figure 7: Generated I/O models for example cell

CONCLUSIONS

To simulate the virtual factory running with the PLC logic code, the counterpart model that receives the PLC output signals and sends the corresponding the signals is necessary. Among the previous approaches for counterpart (plant) model, this paper proposes rapid and efficient method to construct the I/O model. Currently, there is no dominant naming principle for the PLC symbol. By publishing the naming principle of PLC symbol in terms of constructing the I/O model automatically, we can extract the necessary information such as device states, event and operation signals. Even though example cell is simple, we can apply to the larger automated line for the I/O model generation if satisfied that the symbol rule is applied with the proposed naming principle.

The generated I/O model will operate the virtual devices and interfaces the signals with the PLC from the result of the device movement in virtual simulator. The Figure 8 shows the overall feature of virtual simulator that is constituted the generated I/O model and the graphic model.



Figure 8: I/O model and the graphic model of larger scale of virtual factory

In a real factory, the some automatic device doesn't operate in decided sequence. Their operation sequence can be varied and can be complex depend on the neighboring devices. In this case, the I/O model might be complicated and the proposed naming principle is not concerned this limitation. To be the more realistic and practical simulator, however, the I/O model and the corresponding PLC naming principle are needed to cover this issue as the future work.

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OPERATIONS MANAGEMENT BASED ON RFID-IMSII

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KEYWORDS

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ABSTRACT

In order to improve the operations management of a distribution center, this paper proposes a management system based on Multi-Agent Systems (MAS) enhanced with Radio-Frequency Identification (RFID) or RFID-IMSII. An experimental platform composed of a simulation combined with a physical platform is used to study a company situated in Spain. It has been necessary because of the company's complexity. The simulation software WITNESS has been used to study different scenarios. It leads to control the main parameters of the company, for example the schedule of orders. It has been demonstrated that the RFID-IMSII system improves the system utilized by the company.

INTRODUCTION

Distribution centers operate in a competitive environment, which forces them to constantly improve in terms of quality, response, agility and flexibility (Leitao *et al.*, 2008). It could be evaluated in terms of costs by the Life Cycle Cost (LCC); which can be defined as the overall estimated cost for a particular solution considered over its life span. LCC should include direct and indirect initial costs plus any periodic or continuing costs for operation and maintenance (García Márquez *et al.*, 2008). The LCC of a system can simply be considered as the total incurred cost between requirement specification and disposal.

This paper presents a new operations management for a real production company with a distribution center in order to reduce the LCC. It has been necessary to build a physical platform connected to a simulated real facility created by the software GRASP. Web technologies and a network provide communication and actuation in the experimental platform. Modern Programmable Logic Controllers (PLCs) and PCs support the multi-agent systems. Using this platform makes it possible to experiment different techniques without interfering with the company. The traceability has been employed for studying variables of the products, for example its production history. It leads to the creation of a database of the variables (Morel *et al.*,

2007). The identification using radiofrequencies (RFID) leads the traceability control (Finkenzeller, 2004).

The modeling of the movements of parts is at a very detailed level, and it is therefore suited for the analysis of operations which have been carried out in this paper employing discrete simulation (e.g. Law and Kelton, 1991; Pidd, 1998, 2003). The introduction of Visual Interactive Simulation, or VIS, in the late 1970's (Hurrion, 1978) and the move to menudriven model building in the 1980's (Bell, 1989) had a big contribution to the discrete simulation. However, in fairly general terms, most simulationists might agree with a definition of the type: "the use of a model to predict the behaviour of a stochastic system", and perhaps "involving experimentation and statistical analysis of the results".

Indeed the major challenge for the developers of discrete simulation software is to balance flexibility against ease of use: historically the balance was in favour of the former, but the modern emphasis is increasingly on the latter. Surveys appear regularly in the literature (e.g. Swain, 1999) and the choice is exceptionally wide e.g. Arena, Extend, Promodel, Simul8 and Witness. Discrete simulation is now used widely in industry, commerce and the public sector to model the behaviour of systems such as production lines, hospital departments and transport systems. The modeling in a real enterprise case is needed because of its complexity. By using a model, it is possible to manage part of the enterprise, and by some models to manager some parts of the enterprise or to manage all of it.

The model should consider the description, prediction and explanation of the enterprise's work (Flood and Carson, 1993). The description is based on a real case, which is simulated in a laboratory, based on observation. The complexity of the system makes it so that the system cannot be considered to be matched by the predictions obtained through mathematical models. The software Witness will be employed to analyse the data obtained in the laboratory. The analysis is based on past observations for deducing future behavior and it considers the stochastic charasteristic of the system (Casti, 1994). The results obtained by the model should help to obtain an explanation depending on the purpose of the study (Rivett, 1972). Therefore, it is necessary to analyze some key parameters of the business. In this paper a platform is analysed which simulates a real case. It allows design, experiments and evaluates different cases. That is achieved by the Flexible Manufacturing System presented in this work.

FLEXIBLE MANUFACTURING SYSTEM

A Flexible Manufacturing System (FMS) is defined as a manufacturing system that uses extensive automation to integrate the following characteristics (Barros, 2003):

- Processing equipment comprising numerical control machines and robots with the ability to change pieces and tools rapidly.
- Material Handling Systems (MHS), including conveyor belts, fork lifts, elevators, automatic guide vehicles (AGVs) and automatic storage and retrieval systems (ASRSs).
- Sophisticated computerized control and communication systems.
- Efficient management and maintenance structures that can tackle situations such as malfunction.

The MHS can be defined as "A group composed of all of the standard features that make possible the physical movement within the supply chain– including the chain of production and warehouse – of raw materials, work in progress, and finished products" (García *et al.*, 2003). The experimental environment is focused particularly on the operations of materials handling. This is assembled in the facilities of the Autolog Group at the University of Castilla-La Mancha (UCLM, Spain).

MHS has some problems such as: stock control, discrepancies in inventory and complicated processes of picking. It is necessary to apply new technologies in order to minimize these errors in large distribution centers. RFID can manage a lot of information, and it is possible to detect, identify, and verify the nature of the coming products; which allows storing them according to the different rotation levels (Abarca et al., 2007). It is permissible to update the products contained on each pallet at any moment and thus being able to control the quality of operations. RFID allows the products to be marked and inventoried while on conveyor lines, during the loading/unloading of trucks at the docks, or while handling the loads in warehouses or distribution centres (Xiao et al., 2007). It corrects errors in each phase of the supply chain and determines rapidly and precisely the errors produced.

RFID together with Information Management System (RFID-IMS) is understood when an information management system is added to the RFID technology. It can manage every data processed that is being generated in the dynamic systems and to provide that information to the management system (Encinas *et al.*, 2008).

RFID provides the information to the agents. They describe the change in situations in industrial environments, and have the capacity to negotiate and coordinate to achieve a common goal (Franklin and Graesser, 1996). It leads to the adaptation of new technologies that should be able to supply the system with the current information necessary to make decisions online. An agent is also capable of carrying out different objectives through an information exchange in the environment with other human agents or software agents (Garijo, 2002). The decisions made by agents using reasoning are based on their internal knowledge and their experience (Cheeseman *et al.*, 2005).

George *et al.* (1998) proposed an agent model based on beliefs, desires, and intentions (BDI). To characterize these types of agents, the following characteristics are added to the initial definition: beliefs (what it believes to be true), desires (the objective that the agent is trying to reach) and intentions (what it plans to do based on its beliefs to reach its desires).

These properties make the agent applicable to highly dynamic situations, which turn them into promising candidates in providing a management solution. Moreover, software agent technology can monitor and coordinate events, meetings and disseminate information (Balasubramanian et al., 2001) improve Knowledge Management Systems (Soto et al., 2008) and build and maintain organizational memories (Abecker et al., 2003). Other applications have been made in order to improve the manufacturing control and supply network coordination using models of behavior as the one in ant colonies such (Valckenaers et al., 2007).

A multi-agent system (MAS) can be defined as a set of agents that represent the objects of a system, capable of interacting, in order to achieve their individual goals, when they do not have enough knowledge and/or skills to achieve individually their objectives (Leitao *et al.*, 2008).

The MAS model depends on the information available from the elements of the system. Therefore it is necessary to get accurate data to the MAS by a flexible management system. RFID-IMS applied to MASs provide flexibility and intelligent control for its application in production, distribution, storage, etc. The MAS controls the system on-line. The designer only has determine the design characteristics and to implementation. RFID-IMS together with MAS can be defined as an intelligent management system enhanced with radiofrequency identification (RFID-IMSII) (Garcia et al., 2007).

CASE STUDY

The platform is divided into two parts, which together simulate the real system. One is assimilated by a physical platform and other by the 3D visualization environment GRASP. The physical platform simulates the loading/unloading processes. RFID-IMSII technologies have been employed together in a storage and distribution system (see Fig. 1). The program simulates the processes of storage and distribution.



Figure 1: Case study

Platform

The physical platform is shown in Fig. 2. The platform is controlled by the sixth PLC type SIMATIC S7 200. The platform represents the area of the entrance/exit of the products. Tagged pallets arrive to the merchandise loading/unloading zone (loading docks) colored and tagged with RFID. They use different colors to indicate the rotation grade of the products, where red indicates high rotation, yellow medium rotation, green low rotation and blue picking.

Petri nets were used in order to create a generic experimental platform capable of adapting itself to a different distribution center. Petri nets are used for modeling due to their ability to represent small sections of a complex system and it is not need to exert such force trying to model the system. Petri nets are also employed for programming the PLCs.



Fig. 4. Petri net diagram of the processes at the platform

The loading and unloading docks are based on two conveyor belts for the entrance and exit of products. An RFID reader has been installed in the entrance conveyor belt to read the tags of the incoming pallets. It identifies the entering pallet and indicates to the robot arm, Motoman HP3 the position where the pallet should be in the warehouse. The pallets with higher rotation occupy the lowest and closest part to the exit of the automatic warehouse. When the robot has located a pallet, it then connects with the simulation. The pallet will have a route within the automatic warehouse corresponding with the rotation grade of the product and its destination.



Figure 2: Experimental Platform

As as pallet leaves the automated warehouse, the simulation provides the robot with the pallet information. Then the robot transfers the pallet to the exit conveyor belt. After that, the fork-lift takes it to the loading docks. Another RFID reader is located in the exit door in the loading/unloading zone. It verifies the products that are leaving to reduce errors in the entrance and exit of products.

MASs allows the agents to resolve any type of conflict by themselves (Wooldridge, 2002). RFID-IMS II manages the decisions at different places such as: conveyor belt crossing points, entrance and location in the warehouse, and the priority of the orders.

One of the most representative hybrid architectures is the 3-Tiered (3T). It has been develop by NASA (Bonasso, 1997), and it is designed of a multi-agent architecture composed of three levels (Fig. 3): reactive, deliberative and interface.

In the reactive level the agents have the ability to perceive changes in the environment and respond at the same time that the change occurs. The orders are executed without any reasoning, in other words, the agent must decide quickly in critical situations. The simulation that is in this level provides the products' identification and positioning to the system by the interface control level. The reactive level is composed by the following elements: I/O Doors, AGV, Conveyors, Sensors, and Robot.



Figure 3: Multi-Agent Architecture

In the deliberative level, the agents receive the information about their environment and according to their beliefs and intentions, they decide the best way to reach the objectives.

The RFID module assigns one identification code to each pallet and it saves this information in the data capture system, which is a part of the control interface. In addition, it supplies the information to verify the outgoing orders.

The control interface module represents the interface level in the architecture and is composed mainly by Warehouse Management System (WMS), Enterprise Resource Planning (ERP) and the Data Capture System (DCS). Every data generated by the system is stored, decoded, and managed.

The management system's effectiveness depends on accurate and timely information from the data capture system. The control interface transfers data from the reactive level to the deliberative level in both directions. The WMS assigns the position that the pallets will occupy in the warehouse, depending on the level of rotation of the product.

Simulation

The software GRASP 10 has been employed for analyzing the facilities of the biggest Spanish bottling companies. It has been done employing simulations because the investments that should be made in order to correctly automate a production plant or a distribution center are lofty (Coyle *et al.*, 2002). The main investment costs are in the transport equipment made of conveyor belts or cranes, the information systems that control the movement of materials, the software and hardware systems, the formation of human resources, and the most important cost is the design work of the storage process (Otamendi, 2004). The simulation is based on distributed control theory, in other words, it uses the division of a complete system into subsystems with the ability to interact with others and with the intention of achieving a collective objective. It employs a network of Siemens PLCs connected with PROFIBUS DP. It is composed of six PLCs SIMATIC S7 200 (CPU 224) that work as slaves, and a SIMATIC S7 300 (CPU 313C-2DP) that works as master (Fig. 2).

The system is divided into the ground level (inputs), second floor (picking and outputs) and the management of the automatic warehouse (3 S/R Machines). Each part of the system is controlled by a S7 200 PLC and is represented by an agent.

In order to obtain the connection from the PLC network to Ethernet network, a communications processor CP343-1 *Advanced* (Siemens) is added to the master PLC. A computer connected to the network works controlling the interface for the simulation. This interface, programmed in java, serves as a bridge between the decisions made by the PLC network and the simulation. One of the advantages of Ethernet is that it is not necessary that the interface control and simulation are found in the same computer. This makes it possible for a person to supervise the operations that are carried out from any place and control the simulation.

MODEL APPROACH

The agents located at PLCs control the areas of the company simulated by GRASP. The decision of sending a pallet to anyplace is done according to priority. If a pallet k_{ji} from an order \mathbf{K}_j and a pallet k_{rl} from order \mathbf{K}_r arrive to a crossing point in the conveyor belt at the same time, it will selected the pallet that has more priority (Fig. 4).

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_1 \\ \vdots \\ \mathbf{K}_m \end{bmatrix} = \begin{bmatrix} k_{11} \cdots k_{1n} \\ \vdots \\ k_{m1} \cdots k_{mn} \end{bmatrix}$$

ERP provides the priority level relating to the orders that it has in its data base and its current priority considering the pallets that are coming. The priority is determined by the equation (1)

$$P_{k_{ji}} = w_c C_{\mathbf{K}_j} + w_d D_{\mathbf{K}_j} + w_t \mathcal{T}_{\mathbf{K}_j} + \frac{\sum_{i=1}^{j} S_{k_{ji}}}{n}, \quad (1)$$

where $P_{k_{j_i}}$ denotes the priority. $C_{\mathbf{K}_j}$ is the importance degree of a consumer provided by the company, where $0 \le C_{\mathbf{K}_j} \le 1$. $D_{\mathbf{K}_j}$ is the value assigned to the delivery date that is defined by the company, where $0 \le D_{\mathbf{K}_j} \le 1$. $\mathcal{T}_{\mathbf{K}_j}$ denotes the value assigned to the arriving date that is defined by the company, where $0 \leq \mathcal{T}_{\mathbf{K}_{j}} \leq 1$. $S_{k_{ji}}$ is a binary variable that is 0 when the pallet k_{ji} has been not shipped, and in order cases is 1. w_c , w_d and w_t are weights assigned to $C_{\mathbf{K}_j}$, $D_{\mathbf{K}_j}$ and $\mathcal{T}_{\mathbf{K}_j}$ respectively. For example, if a company considers that all the costumers are in the same category, then $w_c = 0$.

The virtual mark V_x that activates the orders to allow pallet k_{ji} to move on to the next process is given by equation (1).

$$V_{x} \begin{cases} P_{k_{ji}} \ge P_{k_{ri}} \Longrightarrow V_{x} = 1 \\ P_{k_{ji}} < P_{k_{ri}} \Longrightarrow V_{x} = 0 \end{cases}$$
(2)

Therefore, according to the above example, the agent, based on the V_x , carries out the decision of which pallet will cross the intersection first.



Figure 4: Prioritization Flowchart

RESULTS

The software Witness has been employed in order to analyse different experiments. A visual interface is shown in Fig. 5.

Witness is a simulation package capable of modeling a variety of discrete (e.g., part-based) and continuous (e.g., fluids and high-volume, fast moving goods) elements. It can be used to simulate the actual production process and provide further information on the operation of the system, such as location of possible bottlenecks and buffer size requirements (Markt and Mayer, 1997).

The company is employing for the order preparations the criteria First Input First Output (FIFO), or First Come First Served (FCFS). To get a flexible system, the criterium employed by the company is not good enough.



Figure 5: Simulation on Witness.

Table 1 shows the characteristics of the reference scheduling and RFID-IMS II are summarized.

Table 1: Reference scheduling vs. RFID-IMSII.

	Reference Scheduling	RFID-IMSII Scheduling
Order Criterium	FIFO	According to priorities
Flexibility	limited	high
Capacity	Fixed	Variable

In order to illustrate the above management system the following case study is presented.

Three incoming orders in the same day have different priority levels:

- 1st Order arrives at 08:00 with low priority.
- 2nd Order arrives at 08:30 with intermediate priority.
- 3rd Order arrives at 09:30 with high priority.

The orders are composed by different amounts of A, B, C and Q products. The last one represents the picking pallets which consist of A, B and C goods. Table 2 shows the description of these orders.

The elaboration times for each order are:

- Order 1: 2h 31' 37''
- Order 2: 2h 16' 36''
- Order 3: 2h 10' 9''

Table 2: Orders' description.

	Order 1	Order 2	Order 3
II.n:4a	11A, 7B,	10A, 8B,	12A, 9B,
Units	5C, 10Q	7C, 8Q	5C, 7Q
Incoming date	13/01/09	13/01/09	13/01/09
Incoming hour	08:00	08:30	09:30
Delivery date	13/01/09	13/01/09	13/01/09
Delivery hour			13:30

Figure 6 shows the Grant diagram for the three orders, where the third order it is not completed on time.



Figure 6. Reference schedule.

Using the management system described in this paper, the total elaboration time obtained is reduced from 6 hours and 51 minutes to 5 hours and 31 minutes. It is reduced by 18.3% of the preparation time. It is possible to fulfill the third order within the delivery time (see Fig. 7).



Figure 7. Schedule obtained by RFID-IMSII.

CONCLUSIONS

A new operations management system has been put to test at a real production company with a distribution center. The company has been analysed by using a physical platform connected with a simulation of a real distribution center. Modern Programmable Logic Controllers (PLCs) and PCs support the deployment of multi-agent systems. They are connected by a network and web technologies provide communication and actuation in the system. The main parameters of the products have been analysed by their traceability. The traceability control has been implemented with RFID.

With the platform design in this paper it is possible to generate, experiment and evaluate different situations of the company. Multi Agent System together RFID-IMS has been used as an intelligent management system (RFID-IMSII).

Discrete simulation is concerned in this paper with modeling the movements of parts at a very detailed level, and it is therefore suited to the analysis of operations. It demonstrates that the RFID-IMSII provides the flexibility necessary to the system to deal with different work orders at the same time. A considerable improvement in the use of the resources is also achieved.

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MODELLING HOT DEFORMATION OF Fe-Ni ALLOYS FOR THE AEROSPACE INDUSTRY

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KEYWORDS

FEM, Fe-Ni-Co alloys, Hot Forging.

ABSTRACT

Hot forging of an Fe-Ni-Co alloy used for aeronautical purposes has been modeled using the commercial software ABAQUSTM/Explicit in order to obtain all the mechanical and thermal information to proceed with piercing and ring rolling. The material used is a 909 Incoloy type super alloy and it is used for the energy generation industry. Information of the constitutive behaviour of the alloy was introduced into the package using experimental data from mechanical testing at different temperatures and strain rates. A thermo coupled analysis was carried out, temperature, stress and strain distributions were evaluated in order to use the results of the model for the further simulation of the ring rolling of the material.

INTRODUCTION

Hot forging of Fe-Ni-Co alloys takes place before piercing and ring rolling, as for other super alloys (Park et al. 1997). The selection of the forging route (temperatures and total strain per step) depends on the requirements of microstructure and final mechanical properties of the product (Cho et al. 2005).

Table 1 shows the chemical composition of the alloy under study and Table 2 its thermal properties. Figure 1 presents the experimental flow behavior of the alloy under mechanical deformation at different strain rates, ranging from 0.001 to 1000, all tests were carried out at a temperature of 1100 °C, other authors have report

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) similar results but for a different material (Sinczak et al. 1998, Thomas et al. 2006).

After forging, piercing takes place, for this particular case a schedule of three steps are necessarily for the piercing, the first step used a tooling to start the hole in the forge piece, a second step includes a correcting tool for the started hole and the last step makes the final cutting. After the piercing has been finished ring rolling continues and sometimes heat treatment to finish with machining. The model here presented includes the forging and the first step of the piercing process.

Table 1: Chemical Composition of Incoloy 909								
Fe Ni Nb Co Al Ti							Si	
Wt%	40.6	38.2	4.80	13.0	0.15	1.50	0.40	

Table 2: Thermal Properties of Incoloy 909 at 1100°C

Thermal Conductivity	16.206 W/m °C
Expansion Coefficient	2.075 E -5 1/ °C
Specific Heat	610 E 6 mJ/ Ton K

FINITE ELEMENT MODEL

The model is designed for hot forging of Fe- Ni-Co alloys prior to piercing and ring rolling operations, hot forging is carried out at 1100 °C, the starting dimensions of the billet are 25.4 and 108.6 cm of diameter and length, respectively, which is deformed 76%, at a forging speed of 0.4cm/s. A 2D dynamic axisymmetric explicit thermocoupled model was developed, using symmetry as to model one quarter of the whole geometry, Fig. 2. The software used for the analysis is Abaqus/Explicit. The model included a total of 2806 nodes and 2674 elements, type CAX4RT, 4-node thermally coupled axisymmetric quadrilateral, bilinear displacement and temperature, reduced integration, hourglass control, mass scaling factor of 100,000 was used. Different friction coefficients at the interface tool-workpiece were used, for the lower tool a coefficient of 0.15 was considered and for the upper tool 0.3 and 0.5. An Adaptive Langrangian Eulerian (ALE) mesh was used. Also convection and radiation to the environment were taken into account for the model, with an emissivity coefficient of 0.7 and convection coefficients of 0.1 for the interface tool-workpiece and 0.01 for the interface workpiece-environment.

Incoloy 909 at T= 1100 C



Figure 1: Mechanical behavior of 909 Incoloy at different strain rates for T=1100°C.



Figure 2: Modeled Geometry, Axial and Radial Symmetry.

The results obtained for the forging are the temperature, the stress and the strain distributions, this information was used in a model to continue modeling the piercing, the ring rolling will be modeled in a further model. The mesh produced after forging was exported as an orphan mesh, which was remeshed, Figure 9. The piercing takes place also at 1100 °C and by three steps, as explained before, only the first step is presented. The piercing is performed in the first step by a tool of 97.5 mm top diameter and 92.5 mm bottom diameter, the time for this step is of 29 seconds, same mass scale factor of 100, 000 was used, also friction was used at the interfase of the upper and lower tools as before, 0.15 and 0.5. For the piercing tool a damage theory was used, same thermal conditions as in forging for convection and radiation were used. A total of 1878 nodes and 1793 elemnts type CAX4RT were included for this model.

RESULTS

Figures 3 to 8 show the results obtained of temperature, equivalent Von Mises stress and plastic strain distributions for the two different values of friction coefficient used, 0.3 and 0.5, at the interface of the upper tool workpiece, the latter gave a slightly bigger concentration of stresses at the tool interface, however at plant process a coefficient of 0.15 is considered, so the presented results must be corrected to the assumed plant value. Also the final dimensions of the billet obtained with the FEM model for the forging are in agreement with those measured at plant, as the final dimensions were constrained.

Results from the piercing model are presented in Figures 10 to 12.

All images presented are generated rotating the 2D axisymmetric geometry.

The speed used for the forging is equivalent to the strain rate of 0.01. The maximum values for the stresses found using μ of 0.3 were of 313 MPa and for μ 0.5 of 315 MPa. A maximum displacement value of 243.3 mm was found for both cases and the maximum temperature was of 1103 °C for both cases.

CONCLUSIONS

A model for the production of forgings for the aerospace industry has been achieved, as well as a model for the first step of the piercing process, further work is needed to obtain the models for finishing the piercing and for the ring rolling, all models must be validated.

It was found that the friction coefficients used do not extern influence on the strain or temperature distribution only on the stress distribution.









Figure 8: Nodal Temperature Distribution using μ 0.5.



Figure 9: a) Orphanmesh after forging using μ 0.5 and b) Remeshed geometry for the piercing model.



-1 185DD62: Step Time = 29.5D 1: S. Mäxes Var: U. Deformation Scale Factor: +1.00De+DD

Figure 10: Stress distribution for the first step of piercing using μ 0.5.



Figure 11: Nodal Temperature Distribution for the first step of piercing using μ 0.5.



Figure 12: Plastic Strain Distribution for the first step of piercing using μ 0.5.

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ANTS SYSTEMS, A STATE OF THE ART OVERVIEW: APPLICATIONS TO INDUSTRIAL PLANTS PROBLEMS

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ABSTRACT

This paper presents a state of the art overview on Ants Systems. Initially the work proposes the fundamental concepts of Ants Theory and offers a description of the main algorithms (based on Ants Theory) and the respective fields of application. Among different fields of application, the paper focuses on industrial plants scheduling problems in open shop, flow shop and job shop systems. The last part of paper discusses about the possibility to combine Modeling & Simulation and Ant Theory to develop advanced real-time support tools for the job shop scheduling problem.

INTRODUCTION

The study of ants' behavior has always interested numerous scientists all over the world. The ability of these social insects to organize and cooperate each other arouses particular interest and curiosity. In particular, Ant's Theory takes inspiration from the observation of ants' behavior when they search for food. In fact, ants are capable of finding the shortest path from source food to their nest and vice-versa, but above all ants are capable of exchanging such information using a simple form of indirect communication (stigmergy). This is possible since ants, while walking from food source to nest, deposit on the ground a particular substance called pheromone, forming a pheromone trail that the other ants can smell. When ants choose the way to follow, they prefer, in probability, paths marked by strong pheromone concentration. In order to better understand ants' behavior we report a n example taken from Dorigo et al. (1996).

In figure 1 ants follow a path between the nest (position in A) and the food (position in E). Suppose that, at certain point in time, an obstacle appears between points A and E. Then, ants have to decide the path to follow: AHE or ACE. As the Figure 2 shows that the two paths are not equal: route AHE is shorter than ACE. Initially ants choose the way to go random: on the average, middle of all ants goes through path AHE and the other half goes through path ACE. Subsequently the choice is influenced by the intensity of pheromone trails that ants smell on the path.

Figure 1: Ants follow a path between points A and E. (Dorigo et al. 1996a)





Ants which choose path ACE spend less time than ants choosing the other path, than the smell of pheromone trails on the first path is more intense than on the longer one (in fact with passing of time pheromone evaporates). Then, ants that return from E to A will find a stronger trail on path ECA and will choose this way. This process continues time after time until all the ants colony will go on the shorter path: ants have been able to identify the optimum tour. It is interesting to note that each ant gives a share for finding the optimal solution, but it is only the ants' colony which finds the shorter path. This is possible using a simple form of indirect communication mediated by pheromone, known as stigmergy (Grassé 1959).

The first author that developed an algorithm based on ants' behavior was Marco Dorigo (Dorigo 1992; Dorigo 1993), followed, after some time, from Luca Maria Gambardella (Gambardella et al. 1997; Gambardella

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) and Dorigo 1995) who proposed several algorithms based on the same principles. While Ant's Theory was spreading, many authors have focused on this research topic, developing algorithms for different fields of application.

Before getting into details of the state of the art overview, in the sequel a brief description of the paper sections is reported. Section 2 proposes a brief description of the main algorithms developed and the respective fields of application. In section 3 the attention is focused on algorithms applied to industrial plants problems (with a description of different cases). Section 4 discusses about one of the most important problems in industrial plants: job-shop scheduling problem. Finally, the last section summarizes conclusions and research activities still on going.

ANT'S THEORY ALGORITHMS

The first model based on Ant's Theory was proposed by Dorigo, it was a new heuristic approach for the solution of combinatorial optimization problems called Ant System (Dorigo et al. 1991; Dorigo 1992; Dorigo et al. 1996). Ant System was first applied to solve traveling salesman problem. Over the years several versions of AS have been developed to improve and extend the performances of the initial algorithm and apply it to solve other optimization problems. In order to develop a common framework for all the versions of the AS, in 1999 was proposed the Ant Colony Optimization (ACO) meta-heuristic (Dorigo and Di Caro 1999a).

Today there are numerous successful implementations of the ACO meta-heuristic applied to different combinatorial optimization problems. It is possible to distinguish two different classes of problems: static combinatorial optimization problems and dynamic combinatorial optimization problems. Static problems are those in which the characteristics of the problem not change while the problem is being solved. On the other hand, dynamic problems are those in which the characteristics of the problem evolve during its resolution. In the following is reported a brief description of the main problems solve with ACO algorithms.

Traveling salesman problem

The first problem solved by an algorithm based on Ant's Theory was the traveling salesman problem (TSP). TSP consists of finding the shortest route visiting each member of a collection of locations and returning to the starting point. At the beginning the algorithm used to solve TSP was the AS, in which the ants build optimum solutions (finding feasible tours of minimum costs) by moving on the problem graph from city to city. Considering the way to update the pheromone trail, three different versions of the AS have been defined: ant-density, ant-quantity and ant-cycle. In the first two versions ants deposit pheromone while building a solution, instead in third version they deposit pheromone only when a complete tour has been built.

The MMAS algorithm (Max-Min AS, Stützle and Hoos 1997a; Stützle and Hoos 1997b) is similar to the AS but, in this version, the pheromone trail is updated offline. The way to update the pheromone trail is the same proposed by Dorigo and Di Caro (1999b): "...the arcs which were used by the best ant in the current iteration receive additional pheromone". The pheromone trail values are restricted at the interval $[\tau_{min}, \tau_{max}]$, and trails are initialized at maximum value τ_{max} .

Another version is the AS_{rank} (Bullnheimer et al. 1997) in which, as in the MMAS version, the arcs that have been visited by ants that carried out the best tour are updates with an additional quantity of pheromone (this is equivalent to AS's elitist ants pheromone updating) The difference is that the ants are ranked by tour length they complete.

The Ant-Q (Dorigo and Gambardella 1995: Gambardella and Dorigo 1996) is an algorithm that tried to fuse the AS and the Q-learning (Watkins 1989). The idea of this algorithm is to update step-by-step pheromone trails with a quantity which is a prediction of the value of the next state. Suddenly it appears that the evaluation of this predictable value was extremely difficult, than Ant-Q was abandoned and replaced by ACS (Ant Colony System; Dorigo and Gambardella 1997a; Dorigo and Gambardella 1997b). The ACS gives approximately the same performances of Ant-Q but it is simpler to use. The two algorithms simply differ in the value used to update pheromone trails.

The ACS is a further version proposed to improve the performance of the AS, that gives good solutions in reasonable time only for small problems. The rationale of ACS and AS is the same but some differences exist:

- In ACS the global pheromone trails are updated offline: at the end of an iteration a quantity of pheromone is added to the arcs used by the ant that complete the best tour;
- Ants use a different decision rule, called pseudo-random-proportional rule, to choose the next city to visit;
- Ants update the pheromone trails only on-line, step-by-step, during the construction of a solution;
- ACS algorithm uses a data structure, called candidate list, that allows to have additional local heuristic information.

Quite similar to ACS is another algorithm: ACS-op-3 (Freisleben and Merz 1996a; Freisleben and Merz 1996b). The difference is that the ACS-op-3 activates a local search procedure (based on variant of the 3-opt local search procedure) to improve the solutions generated by ants.

Quadratic Assignment Problem

QAP is the problem to assign n resources to n locations trying to minimize total allocation cost (this cost is a function of the way to allocation chosen). This kind of problem is a generalization of TSP. As a consequence the algorithms used to solve a QAP are generalization of algorithms used to solve the TSP. Further information can be found in Maniezzo et al. (1994) that propose the AS-QAP algorithm and in Stützle and Hoos (1998) that propose the MMAS-QAP algorithm.

Job scheduling problem

The problem is the following: given M machines and a set of J jobs it is necessary to choose the order sequence of operations to be executed on these machines so that the maximum of the completion times of all operations is minimized and no two jobs are processed at the same time on the same machine. The algorithm used to solve this problem is the AS, but since exist some differences in nature of the constraints of this problem respect to the TSP, it is necessary to define a new way of building the ants' tabu list. Currently AS-JSP algorithm (Colorni et al. 1994) is used to solve problems of maximum dimensions up to 15 machines and 15 jobs and the generate results are not satisfactory. This results suggest that this field of applications should be further investigated.

Vehicle Routing

Vehicle Routing problem is the following: consider a graph G=(N,A,d), where N is the set of nodes, A is the set of arcs and d_{ij} is a weight associated to arc (i,j) that represent the distance between node i and j. Node 0 represents a deposit in which are localized vehicles (each one of capacity C), while the other nodes represent customers that should be served and ask a quantity D at time T. The problem is to find the cycle of minimum cost such that every customer is visited and its demand dispatched respecting vehicle capacity constrains and assuring that every vehicle starts and ends its tour in the depot. The first algorithm proposed for this problem is AS-VRP that is an extension of the AS based on AS_{rank}. Another algorithm for the Vehicle Routing problem is HAS-VRP (Gambardella et al. 1999). This algorithm first reformulates the initial problem by adding to the city a set of M-1 depots, where M is the numbers of vehicle. In this way the initial problem becomes a TSP with additional constraints. Then it is applied HAS-VRP algorithm, which is inspired by ACS. Specific research works in the field of vehicle routing have also been developed by De Sensi et al. (2006) and Curcio et al. (2007). The first research work presents an AS algorithm integrated in a simulation model for supply chain vehicle routing optimization. The second one compares the AS and

Genetic Algorithms (GA) for vehicles routing optimization in a pharmaceutical distribution system.

Sequential Ordering

The sequential ordering problem consists in finding minimum weight Hamiltonian cycle on a directed graph with nodes and arcs weighted and trying to respect precedence constraints among nodes. In this case the proposed algorithm is HAS-SOP (Gambardella e Dorigo 1997), an extension of ACS. In fact, in HAS-SOP, unlike ACS, the set of feasible nodes is built taking in consideration the precedence constraints and, for local search, it is use a variant of 3-opt procedure.

Graph Colouring

Graph Colouring is the problem to find minimum number of colours for colouring a graph. The algorithm proposed is ANTCOL (Costa and Hertz 1997) that makes use of well-known graph colouring heuristics *recursive large first* (RLF) (Leighton 1979) and DSATUR (Brelaz 1979).

Shortest Common Supersequence

The shortest common supersequence (scs) is a common supersequence of minimal length given two sequences $A = \langle a_1, ..., a_m \rangle$, $B = \langle b_1, ..., b_n \rangle$. In the shortest common supersequence problem, the two sequences **A** and **B** are given and the objective is to find the shortest possible common supersequence of these sequences. In general, the scs is not unique. This problem is solved by an algorithm called AS-SCS (Michel and Middendorf 1998), which differs from AS classic because AS-SCS uses a look-ahead function which takes into account the influence of the choice of the next symbol to append at the next iteration.

Algorithms for dynamic combinatorial optimization problems

Table 1 lists all the algorithms presented in the previous sections also reporting authors and field of application. The algorithms for dynamic combinatorial optimization problems have focused on communications networks. In fact, this kind of problem is characterized by dynamic conditions. ACO implementations for communications networks are grouped in two classes: connection-oriented and connection-less networks. In the first case all the packets follow a common path in a preliminary phase of selection, instead in the second one all packets can follow different paths. Algorithms proposed for the two classes are reported in the next table (Table 2) with a list of references.

Table 1: List of applications of ACO algorithms to static combinatorial optimization problems (Dorigo and Di Caro 1999).

Problem Name	Authors	Algorithm Name
	Dorigo, Maniezzo & Colorni, 1991	• AS
	Gambardella & Dorigo, 1995	• Ant-Q
Traveling Salesman	Dorigo & Gambardella, 1996	ACS & ACS-3-opt
	Stützle & Hoos, 1997	• MMAS
	Bullnheimer, Hartl & Strauss, 1997	• AS _{rank}
	Maniezzo, Colorni & Dorigo, 1994	• AS-QAP
	Gambardella, Taillard & Dorigo,	• HAS-QAP
Quadratic	1997	• MMAS-QAP
Assignment	Stützle & Hoos, 1998	• AS-QAP
	Maniezzo & Colorni, 1998	ANTS-QAP
	Maniezzo, 1998	
Job-shop Scheduling	Colorni, Dorigo & Maniezzo, 1994	• AS-JSP
	Bullnheimer, Hartl & Strauss, 1996	• AS-VRP
	Gambardella, Taillard & Agazzi,	• HAS-VRP
Vehicle Routing	1999	• AS
	De Sensi et al., 2006	• AS & GA
	Curcio et al., 2007	
Sequential Ordering	Gambardella & Dorigo, 1997	HAS-SOP
Graph Coloring	Costa & Hertz, 1997	ANTCOL
Shortest Common Supersequence	Michel & Middendorf, 1998	• AS-SCS

Table 2: List of applications of ACO algorithms to dynamic combinatorial optimization problems (Dorigo and Di Carlo 1999)

Problem	Authors	Algorithm Name
Name		
	Schoonderwoerd, Holland, Bruten &	• ABC
Connection-	Rothkrantz, 1996	
oriented	• White, Pagurek & Oppacher, 1998	• ASGA
network	• Di Carlo & Dorigo, 1998	AntNet-FS
routing	Bonabeau, Henaux, Guérin, Snyers, Kuntz &	ABC-smartants
	Théraulaz, 1998	
	Di Carlo & Dorigo, 1997	AntNet & AntNet-
Connection-		FA
less	Subramanian, Druschel & Chen, 1997	Regular ants
network	Heusse, Guérin, Snyers & Kuntz, 1998	• CAF
routing	Van der Put & Rothkrantz, 1998	ABC backward

The next section focuses on ants' algorithms developed for specific applications in industrial field.

ANT'S THEORY APPLIED TO PRODUCTION SCHEDULINGS IN INDUSTRIAL PLANTS

The problem of production scheduling within industrial plants consists of scheduling jobs (i.e. shop orders) on the available machines over the time. The production scheduling problem allows multilevel classification:

- 1) Depending on the number of machines:
- <u>Scheduling on single machine</u>: in this case it is necessary to find the sequence of jobs that minimize use time of a single machine (in literature known as "problems of pure scheduling);

- <u>Scheduling on multi-machines</u>: in this case jobs should be processed on more machines.
- 2) The scheduling on multi-machines can be also divided in:
- <u>Scheduling on homogeneous machines:</u> all machines execute the same operation and jobs can be processed indifferently on each machine. The problem is twofold: assignment of each job to one of the alternative machines (first level: assignment problem); jobs scheduling on each machine (second level: scheduling problem), with the aim to optimising an objective function.
- <u>Scheduling on heterogeneous machines</u>: each machine executes a particular operation.
- For jobs scheduling the following case have to be considered:
- <u>Open shop</u>: jobs do not have a fixed machines visiting order;
- <u>Flow shop:</u> jobs have to be processed through a fixed sequence of machines and the processing operation order of each job is the same.
- <u>Job shop:</u> jobs have to be processed through a sequence of machines, but the processing operation order as well as the sequence of machines of each job is different from other.

The following figure 3 represents schematically the previous scheduling problems classification within industrial plants. In the following we focus the attention first on single machine problem and then on the last three problems (open, flow and job shop) and, in particular, we present the ACO algorithms proposed to solve these problems.



Figure 3: Classification of production scheduling problems.

Single Machine

In this case jobs utilize the same resource (machine). In a real world system (i.e. an industrial plant) several elements make this problem very complex: process time, due date, and above all setup time. In literature, we find that this problem has been classified as NP-hard and its description is as follows: there are n jobs to be processed on the same machine; the machine can process only one job at a time. Each job is characterized by: processing time, due date, weight in terms of cost for time unit and setup time. To solve this problem an ACO heuristic has been presented by Liao & Juan (Liao & Juan 2005). The ACO algorithm proposed by Liao & Juan is basically the ACS version but it introduces the minimum pheromone value from "max-min-ant-system" (MMAS). The algorithm has two additional distinctive features: it introduces a new parameter for the initial pheromone trail and adjusts the timing of applying local search.

Another ACO algorithm for the same problem was proposed by Gravel (Gravel et al. 2001). In this case the algorithm is developed on a real industrial case study: a scheduling problem in an alcan aluminum foundry. In this algorithm the ACO meta-heuristic allows to perform a multi-objective optimization: minimization of unused capacity, minimization of the total tardiness of the set of orders, minimization of the total number of required when changing draining materials, minimization of transportation function penalty that computes the total unused vehicle capacity. To adapt the algorithm the authors implement a distance matrix D that contains information derived from each of the objectives and, on the other hand, a new rule for updating the pheromone trail at the end of a cycle based on one of the objectives.

Open Shop

The Open Shop problem can be defined as follows: a finite set of jobs, O, that have to be processed on a set of machines, M. Jobs do not have a fixed order to visit machines and each machine can process one job at a time. The objective is to minimize the makespan (the maximum of jobs completion time).

The algorithm proposed to solve this problem, based on Ant's Theory, is Beam-ACO (Blum, 2005). This algorithm is an union between Ant Colony Optimization and Beam Search (Ow PS 1988), a classical tree search method that is a derivation of branch and bound algorithm. Beam-ACO works as follows: for each iteration, n ants perform a probabilistic beam search and each ant constructs up to k solutions. Then, depending on a measure, called convergence factor, and a boolean control variable, an update of the pheromone values is performed. After, the convergence factor is recomputed and it is decided if the algorithm has to be restarted. The algorithm stops when the termination conditions are satisfied.

Flow Shop

The simplest case of Flow Shop is the 2-machine flowshop scheduling problem with n jobs to schedule

on 2 machines. Every jobs have a specific processing time on the two machines (i.e. job *i* has processing time a_i on first machine and b_i on second machine). C_i is the completion time of job *i* on machine 2, where i=1,...n. For these types of problems two criterions can be defined: (i) the makespan criterion, called Cmax, defined as the maximum completion time of jobs on machine 2; (ii) the total completion time criterion, called ΣCi , defined as the sum of completion time of jobs on machine 2. It is supposed that the total completion time criterion has to be minimized subject to the condition that the makespan computed is minimum. It is supposed to minimize the makespan (maximum completion time) as the primary objective and minimize total flow-time (sum of the completion times of all jobs) as the secondary objective. In practice this problem is a multiple criteria scheduling problem and it is a strongly NP-hard.

The 2-machine flowshop scheduling problem has been extensively studied in literature and both exact and heuristic algorithms have been proposed. An ACO algorithm was also proposed to solve this problem.

The ACO heuristic proposed for this problem is known as SACO (T'kindt et al. 2001). In SACO each ant builds a feasible schedule by using a constructive procedure. This procedure uses a particular structure called "pheromone matrix" that, based on memory shared by ants, contains the information about the ways to build a good feasible schedule. Every element that composes the pheromone matrix represents a probability (i.e. τ_{ii} is the probability of having job i at position j in a good schedule for the \sum Ci criterion). Starting from position 1 to position n, the most suitable job for position j is chosen according to either the intensification mode (the ant chooses the job with the highest value of τ_{ij}) or the diversification mode (the ant uses a wheel process to select the most suitable job). When an ant has built a complete schedule, a local search is applied, that among various schedules keeps the schedule that has an optimal value of the makespan and the lowest value for the total completion time. Several computational experiments have suggested that SACO yields better results than existing heuristics.

Another variant of 2-machine flowshop scheduling problem involve the machine setup time. In this case the objective function is to find a schedule of jobs such that the total completion time, the sum of completion times of all jobs, is minimized. To solve this problem was proposed a particular variant of ACO (Shyu et al. 2004). First of all the original problem is transformed into a graph-based-model in which every edge has an associated weight w. Also, unlike the strategy used by Dorigo in classical ACO, where every edge has a constant quantity of initial pheromone, this method initializes the pheromone on edges on the basis of results obtained by a greedy heuristic algorithm. To obtain a better initialization of pheromone intensity, the greedy heuristic is applied *n* times by letting every node be the starting node. Obtained the initial solution the algorithm starts choosing the next node to visit and updating pheromone trail. The algorithm ends after a given number of iterative cycles.

The flow shop problem becomes more complicate in case of n machines. Rajendran & Ziegler (2002) propose two algorithms to solve this problem. The first algorithm, called M-MMAS, extends the ant-colony algorithm called MMAS, by incorporating the summation rule developed by Merkle and Middendorf (2000) for the single-machine total weighted-tardiness problem, and modifying the procedure for job selection to be appended to the partial ant-sequence. In addition, the M-MMAS makes use of a new local search technique, called job-index-based local search. The second algorithm developed by Rajendran & Ziegler (2002) is called PACO. The first sequence of the antcolony algorithm is obtained in a way similar to M-MMAS with the objective function value set to best value. There is a specific procedure to select an unscheduled job i for position k. The resulting sequence is subjected to the job index-based local search scheme three times to improve the solution. Moreover the algorithm has a procedure to update pheromone trail based, not only on the resultant sequence obtained after the three-time application of the job index-based local search procedure, but also on the relative distance between a given position and the position of job *i* in the resultant sequence. PACO algorithm generates 40 antsequences and among them it is obtained the best heuristic sequence.

Another important contribution is the application of ACS to solve flow shop problem, in which n jobs should be processed on m machines, with the objective to find a permutation of jobs that minimizes the makespan. The problem can be represented in ACS by a disjunctive graph, where the set O contains all operations of each job on machine, C contains the precedence relationships between the processing operations of a single job, and D represents the machine constraints of operations belonging to different jobs. Also, there are two additional nodes: a nest node N and a source food node F. After the construction of the graph, since the jobs have all the same ordering sequence, it is simple to find the first sequence. The next node an ant chooses to move to is calculated by applying a specific state transition rule. The chosen node is then added to the tabu list and the process is iterated. At the end, the node permutation given by the tabu list can determine the job sequence.

Another algorithm to solve the flow shop scheduling problem was proposed by Gajpal et al. (2005), called NACO. This time the aim is to minimize the variance of jobs completion times (called the completion-timevariance problem, CTV). In the NACO algorithm the initial solution is obtained by NEH (Nawaz, Enscore and Ham) heuristic considering the jobs CTV minimization. To improve the initial sequence is used a random-job-insertion local search procedure and for every ant-sequence generated and for final solution is executed the local search procedure three times. As in every ACO algorithm, there is a step to update the pheromone trail or trail intensity.

Job Shop

Among different scheduling problems previously presented the job shop is the most difficult and problematic to handle. Nowadays most of the industries, developing FMS (Flexible Manufacturing Systems), have to deal with job shop scheduling problem. As a consequence numerous algorithms and procedures have been developed over the time to handle this problem. In the last years also algorithms based on ACO metaheuristic have been proposed.

The first algorithm handles the problem of FJP (flexible job shop scheduling) which extends the classic problem of job-shop scheduling. In fact, in a very large number of industries all available machines are divided into groups of identical machine tools. This version of job shop scheduling problem is known as FJS with parallel machines. A scheduling algorithm was introduced by Rossi and Dini (2006) and represents the FJS problem with separable transportation and sequence dependent setup times in a disjunctive graph. The aim of the algorithm is to minimize the makespan. The algorithm proposed is ACS with a number of innovative skills: the first is an approach based on the disjunctive graph model and a LS (List Scheduler) algorithm (that drives an ant to visit the digraph model). The second feature is the pheromone trail structure that is based on the before mentioned disjunctive graph model. Finally, two original components, the routing-precedence-based visibility function and the method to approximate nondelay schedules are introduced to improve the performance.

For FJS problem another important procedure have been obtained combining GA (genetic algorithm) with ACO (Rossi & Boschi 2008) as a mechanism of collaborative search. This procedure presents new skills in the methods of selecting the GA subpopulations and updating pheromone trails. This algorithm has been implemented in a real system to test its performances; the results show that the algorithm is a powerful mechanism for enhancing the searching capability of both genetic algorithms and ant colony systems.

ACO AND MODELLING AND SIMULATION

This paragraph discusses about simulation use in job shop scheduling problem (in real industrial environments) and in particular about the implementation of simulation models supported by ACO meta-heuristic.

The job shop scheduling problem within real industrial environments is usually characterized by a number of restrictive assumptions (i.e. complete resources utilization, no preemption, a job cannot simultaneously occupy more than one machine at a time, etc.). Restrictive assumptions generate ideal scenarios, useful to gain confidence and knowledge about the real system, but they do not give the possibility to transfer and apply final results to the real system. Usually restrictive assumptions can be deleted using Modeling & Simulation to recreate systems complexity.

In the following we report an example of simulation model to solve the flexible job shop scheduling problem. This work, proposed by Li-Ning Xing et al. (2008), considers the following restrictive assumptions for the job shop scheduling problem:

- Jobs are independent from each other;
- Machines are independent from each other;
- Setting up time of machines is negligible;
- Move time between operations is negligible;
- At a given time, a machine can execute at most one operation;
- No more than one operation of the same job can be executed at a time;
- There are no precedence constraints among the operations of different jobs.

The aim of a simulation model is to assign the operations to machines and to schedule the operations on each machine according to certain rules (i.e. scheduling rules) or algorithms (i.e. genetic algorithms, ACO algorithms).

In the past, the authors have already introduced Modeling & Simulation (M&S) for supporting production scheduling in real industrial plants (in particular job shop systems). Longo et al. (2003) presents a simulation model for shop orders scheduling in special glass manufacturing; Longo et al. (2006-a) use M&S combined with scheduling rules for production planning within a manufacturing plant devoted to produce high pressure hydraulic hoses. Longo et al. (2006-b) face the scheduling problems (and plant layout optimization) in a wood frames manufacturing process. Finally Longo et al. (2008) combine M&S and genetic algorithms for shop orders scheduling in a real manufacturing plant.

AN APPLICATION EXAMPLE

This section presents the initial results of a research work (developed by authors) that aims at using Modeling & Simulation in a job shop scheduling problem supported by ACO meta-heuristic.

The job shop system manufactures high pressure hydraulic hoses (Longo et al., 2006-a). Each product is made up by a high pressure hose, two adapters and two hydraulic fittings. The production process is made up by 8 different operations:

- Materials preparation
- Fittings stamp
- Hoses cutting
- Hose skinning
- Assembly
- Junction
- Hydraulic hoses Testing
- Final controls and packaging

Two types of Shop Orders (S.Os) can enter the system: normal S.Os and priority S.Os. Usually normal S.Os are scheduled on a 2-weeks time window (each new S.O. enters in the last position of the 2-weeks queue). On the contrary, a priority S.O. can enter the 2-weeks queue in any position at any time (it depends on the priority level of the S.O.). In other words the system allows the *passing* between jobs. Each S.O. has a finite number mof operations, one on each machine and it is allowed to work twice a job on the same machine. All the S.Os entered into the system must be necessarily completed.

Machines could not be available during the scheduling period because of the failures. Failures have been modeled by using a negative exponential distribution for both the Mean Time to Failure (MTTF, expressing the time between two consecutive machine failures) and the Mean Time to Repair (MTTR, expressing the time required for repairing the machine). Finally process and set-up's times are considered as stochastic variables each one with a specific distribution form based on historical data. According to these hypotheses it follows that the case analysed belong to the *dynamic-stochastic* scheduling problem because new S.Os arrive during the scheduling horizon and most of the numerical quantities are stochastic.

The simulation model of the job shop system was developed by using the discrete event simulation software eM-Plant. The figure 4 shows the main frame of the simulation model.



Fig. 4 – Simulation model main frame

Further implementations have been carried out to introduce an Ant System algorithm as support tool for S.Os scheduling. The implementation of the algorithm as well as the interface with the simulation model was created through the programming of specific subroutines, written using the simulation language Simple++.

Some initial optimizations have been carried out trying to minimize the S.Os flow time and lateness and maximize the fill rate (the last one intended as percentage of S.Os that meet the due date). The flow time reduction was about 10.5% lower than the best result obtained by using the Short Production Time (SPT) scheduling rule. Analogously the lateness reduction was about 13.4% lower than the best solution obtained by using the Due Date scheduling rule. Finally the fill rate improvement was about 5.1% greater than the best solution obtained by using the Due Date scheduling rule.

CONCLUSIONS

The paper presents a state of art about Ants System with particular attention to industrial plants problems. The state of art shows that the main fields of application for ACO algorithms are the routing problems, but in the last years, different applications have been developed to solve industrial plants problems and, in particular, production scheduling problems (job shop, flow shop, open shop). The final part of the paper focuses on the integration of Modeling & Simulation and Ant Theory for supporting real time production scheduling in job shop systems. The authors present some initial results on the development of a simulation model of a real industrial plant (job shop system) supported by an AS algorithm. Further researches are still on going for simulation model accreditation within the real system in order to use it a support tool for real-time production scheduling.

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Finance and Economics

COMMODITIES PRICES MODELING USING GAUSSIAN POISSON-EXPONENTIAL STOCHASTIC PROCESSES, A PRACTICAL IMPLEMENTATION IN THE CASE OF COPPER

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KEYWORDS

Commodities prices modelling, Gaussian Poisson, Exponential Processes.

ABSTRACT

Due to an assignment, received from a Chilean mining company, to value a copper mine with an estimated life span of several decades, we implemented a model of copper prices using mean reversion with Gaussian Poisson exponential jumps.

The parameters of the model are extracted from the copper prices series. The exponential distributions of the jumps are estimated via a standard simulation program using best likelihood methods.

Until the model was implemented, the company had been using a long term mean price to estimate mining projects' cash flows. This approach had worked satisfactorily given that, as shown in the Chart 1, the average price of copper had ranged around 100 cents of USD per pound between 1996 and 2004.



Chart 1. Daily copper prices from January 1996 to January 2009. Source: Cochilco

However, a turnaround in the cycle occurred in 2004, with prices going up between that year and 2008 to reach

a mean value of 325 ç/pound. At the end of 2008 the price dropped down up to the level of 150 ç/pound. The prices series analysis suggests the existence of mean reversion with stochastic jumps especially from 2006.

INTRODUCTION

Mean reversion models originally proposed by (Ornstein & Uhlenbeck 1930) are predicated on the notion that the long-term behavior of prices gravitates towards a mean price.

The price adjustment mechanism is accounted for by market forces, in that –leaving aside speculative movements in financial markets, which in specific cases can be the cause of price volatility- the market adjusts itself in periods of strong demand and rising prices through an increase in the offer, e.g. by opening up closed mines, by extending the life span of mines scheduled to be shut down, etc. Following this increase in the offer, prices tend to fall. In periods when prices are low, the opposite occurs, so that the offer decreases and prices tend to go up.

(Dixit & Pindyck 1994) suggest the use of the mean reversion model to model the behavior of commodity prices and propose a model that will be used in the paper.

The model of Poisson jumps for the securities prices was proposed by (Press 1967). (Merton 1976) proposes a model of geometric Brownian motion with jumps which characterizes the jumps as the arriving of new important information. Merton makes an important improvement to the model adjusting the Poisson process to convert it to a Martingale.

(Das 1998) uses a model of mean reversion with exponentially distributed Bernoulli Poisson jumps for modeling interest rates developing an analytical formula for the parameterization of the model.

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) (Dias & Rocha 2001) applies the (Dixit & Pindyck 1994) model with Gaussian distributed Poisson jumps for modeling petroleum prices. The important contribution of (Dias & Rocha 2001) is the specification of the discrete model for the simulation although they make a simplification because they apply the same probability of jumps up or down using a Gaussian distribution for the size of the jump.

In our case we will use the (Dixit & Pindyck 1994) model adapted by Dias & Rocha, but deriving ourselves the discrete simulation formula of exponentially distributed Bernoulli Poisson jumps.

MEAN REVERSION MODELS OF PRICES

A given random variable, X_T , responds to the following stochastic differential equation:

$$dx = \eta \left(\overline{x} - x \right) dt + \sigma dz \tag{1.1}$$

With \overline{x} being the expected mean price, x the current price, and η a reversion speed parameter that will be explained below.

Formula (1.1) tells us that dx tends to be negative when $\overline{x} < x$ -that is, when the mean price is smaller than the current price-, thus meaning that the change tends to push prices down. However, when $\overline{x} > x$, the mean price is higher than the current price, and dx tends to represent a positive change that pushes the price upward.

The speed of reversion is given by parameter η , a reversion process's mean life is the time it takes for the price to cover half the distance that separates it from the mean price. In other words, a mean life of one year means that it takes two years for the price to reach its mean value.

The relationship between mean life, H, and reversion speed, η , is:

$$H = \frac{\log(2)}{\eta}; \qquad \eta = \frac{\log(2)}{H} \tag{1.2}$$

The solution of (Kloeden & Platen 1992) for the stochastic differential equation (1.1) in terms of Ito's stochastic integral is as follows:

$$x_{T} = x_{0}e^{-\eta T} + (1 - e^{-\eta T})\overline{x} + \sigma e^{-\eta T} \int_{0}^{T} e^{\eta t} dz$$
(1.3)

As pointed out by (Dixit & Pindyck 1994), the mean and the variance of the X_T variable are given by the following expressions:

$$E(X_T) = x_0 e^{-\eta T} + \overline{x} \left(1 - e^{-\eta T} \right)$$

$$Var(X_T) = \left(1 - e^{-2\eta} \right) \frac{\sigma^2}{2\eta}$$
(1.4)

Since X_T follows a distribution which may take negative values, we will define $x = \log(S)$ and $S = e^x$, with S being the asset price.

The variance needs to be adjusted by $\frac{1}{2}$ in order to obtain the exact formula for the simulation, which will thus be:

$$S_{t} = e^{\left(\log(S_{t-1})e^{-\eta\omega} + \log(\bar{S})(1-e^{-\eta\omega}) - (1-e^{-2\eta\omega})\frac{\sigma^{2}}{4\eta} + \sigma\sqrt{\frac{1-e^{-2\eta\omega}}{2\eta}}dz\right)}$$
(1.5)
$$dz \sim N(0,1)$$

where the first two terms on the right-hand side are the process's drift terms that weigh the initial value and the mean value of equilibrium. The third term is an adjustment term required by Jensen's inequality, and the fourth term is the variance term multiplied by a Wiener stochastic process that draws values from a N (0,1) distribution.

MEAN REVERSION MODEL WITH POISSON EXPONENTIAL JUMPS

Mathematically, a mean reversion process with jumps is formulated by adding a new term to the mean reversion's stochastic differential equation:

$$dx = \eta \left(\overline{x} - x\right) dt + \sigma dz + dq \tag{1.6}$$

The dq term is a Poisson term whose value is zero most of the time; yet λ often takes a value that prompts a jump in the variable $x = \log(S)$.

$$dq \begin{cases} 0 & with \ probability \ 1 - \lambda dt \\ 1 & with \ probability \ \lambda dt \end{cases}$$
(1.7)

Should there be up jumps with a frequency λ_u and down jumps with a frequency λ_d , then:

$$\lambda = \lambda_{\mu} + \lambda_{d} \tag{1.8}$$

So that dq is the jump-size distribution when such jumps are up or down (ϕ_{a}, ϕ_{d}) .

We start from the assumption that the mean reverting process, dz, and the Poisson process, dq, are not correlated.

The jump's size and direction are random, and $k = E[\phi]$

is the expected value of the joint distribution (ϕ) for up jumps and down jumps.

In order for the expected value of the dx process to be independent of the jump parameters, it needs to be compensated by subtracting from it the term λk . We thus use a compensated Poisson process and eliminate the trend that might incorporate into the process the effect of a higher number of up or down jumps. Hence, the modified formula is:

$$dx = \left[\eta\left(\overline{x} - x\right) - \lambda k\right]dt + \sigma dz + dq \tag{1.9}$$

The mean of X_T now becomes:

$$E[X_T] = xe^{-\eta} + (\overline{x} + \lambda k\eta)(1 - e^{-\eta})$$
(1.10)

Note that when the expectation of the jumps is k = 0, this last expression is identical to the expectation of X_T in a mean reversion process without jumps, confirming that the possible trend introduced by the jumps has indeed been eliminated.

The variance of the mean reversion process with jumps is:

$$Var(X_{T}) = \frac{\sigma^{2} + \lambda Var(\phi)}{2\eta} (1 - e^{-2\eta})$$
(1.11)

We adjust the solution of the process by including the variance term of the Poisson distribution for up and down jumps:

$$S_{t} = e^{\begin{pmatrix} \log(S_{t-1})e^{-\eta \Delta t} \\ +\log(\overline{S}+\lambda k\eta)(1-e^{-\eta \Delta t}) \\ +dq - (1-e^{-2\eta \Delta t}) \frac{\sigma^{2} + (\lambda_{u} + \lambda_{d}) Var(\phi)}{4\eta} \\ +\sigma \sqrt{\frac{1-e^{-2\eta \Delta t}}{2\eta}} dz \end{pmatrix}}$$
(1.12)

For the simulation of the S_t variable, which follows a mean reversion process with jumps, we use the following formulas:

$$x_{t} = \log(S_{t-1})e^{-\eta\Delta t} + \log(\overline{S} + \lambda k\eta)(1 - e^{-\eta\Delta t})$$

$$+\sigma\sqrt{\frac{1 - e^{-2\eta\Delta t}}{2\eta}}dz + dq$$
(1.13)

and:

$$S_{t} = e^{\left(x_{t} - \left(1 - e^{-2\eta \Delta t}\right)\frac{\sigma^{2} + \lambda Var(\phi)}{4\eta}\right)}$$
(1.14)

 $\lambda = \lambda_u + \lambda_d$ is the sum of the frequencies of up jumps and down jumps, respectively, and $Var(\phi)$ is the variance of the jump process that we will be obtained directly from the market data.

To simulate the occurrence of a jump, the expected frequency of up jumps and down jumps per time unit is compared, for each period, with a random value obtained from a [0,1] uniform distribution. If the value drawn in the random extraction is $u < \lambda_u dt$, then a jump up is assumed, and dq takes its value. If, on the contrary, $u < \lambda_d dt$, then a jump down is assumed, and dq takes its value.

Calculating the mean reversion parameters

(Dixit & Pindyck 1994) described how to estimate the mean reversion parameters, building on the idea that the mean reversion's partial differential equation

$$dx = \eta \left(\overline{x} - x \right) dt + \sigma dz \tag{1.15}$$

matches the following AR (1) discrete-time autoregressive process:

$$x_{t} - x_{t-1} = \overline{x} \left(1 - e^{-\eta} \right) + \left(e^{-\eta} - 1 \right) x_{t-1} + \varepsilon_{t}$$
(1.16)

Where ε_t follows a normal distribution with standard deviation σ_{ε} , and:

$$\sigma_{\varepsilon}^{2} = \frac{\sigma^{2}}{2\eta} \left(1 - e^{-2\eta} \right) \tag{1.17}$$

Hence, the parameters of equation (1.17) may be estimated using market price data by means of the following regression:

$$x_{t} - x_{t-1} = a + bx_{t-1} + \varepsilon_{t}$$
(1.18)

Which allows us to determine the mean reversion parameters:

$$\overline{x} = \frac{-\hat{a}}{\hat{b}},$$

$$\hat{\eta} = -\log(1+\hat{b})$$
(1.19)

We take (1.17) as a measure of the reversion process volatility, with σ^2 being the variance of the price series return figures.

The Data

We use copper price data from January 1996 to January 2009. The series consists of 3305 daily price figures. These observed data span a period of 13 years.

Following the Dixit & Pindyck model (1994), we assure that the mean reversion model is adequate and make the Unit Root Test accepting the hypothesis that the series has a unit root and is not a random walk, in other words, the x_{t-1} term is significantly different from 0 as can be seen in Table 1:

Null Hypothesis: COPPER_PRICE has a unit root Exogenous: Constant Lag Length: 1 (Automatic based on SIC. MAXLAG=28)

ag Eengin. T (Automatic based on oro, MAXEAO-20)							
		t-Statistic	Prob.*				
Augmented Dickey-Fi	uller test statistic	-0.980970	0.7620				
Test critical values:	1% level	-3.432142					
	5% level	-2.862217					
	100/ loval	0 667174					

*MacKinnon (1996) one-sided p-values.

Table 1. Unit Root Test of the prices series.

We use the log of the prices series to estimate the regression parameters $\hat{a} = 0.002214$, $\hat{b} = -0.000455$ and $\varepsilon = 0.0177112$, using these parameters to determine the reversion values given by Dixit and Pindyck's (1.19) formula, and we arrive to the results of Table 2.

$$\overline{x} = -\frac{0.002214}{-0.000455} = 4.86508; \quad \overline{P} = e^{(4.85508)} = 129.68$$
$$\hat{\eta} = -\log(1 - 0.0004551) = 0.000452 \implies Mean Life = \frac{\log(2)}{0.000452} = 1522 \, days$$
$$\hat{\sigma} = \sqrt{\frac{(0.017711)^2}{2(0.0004552)} (1 - e^{-2(0.0004552)})} = 0.0125236$$

Table 2. Mean reversion formulas and parameters.

We obtain a mean price of 129.68 c/pound. The estimated mean life of 1522 days correspond to a mean life of 6 years entails that the series goes back to its mean approximately every 12 years.

As for the standard deviation, we notice that it tends to 0.01252, which is lower than its value in the original series (0.01771).

Estimating the jump distribution

We will estimate the parameters of the jump distribution on the basis of (Clewlow & Strickland's 2000) work considering that values of more than 3 standard deviation are jumps in the series as can be seen in Chart 2.



Chart 2. Returns of the daily copper prices and the ± 3 standard deviation limits.

In order to isolate the jump component, we subject the returns to a recurrent filtering. The methodology is as follows:

- 1. We analyze the series and take out the returns located above or below the 3 standard deviation limits.
- 2. We analyze the series again and similarly take out the returns above or below 3 standard deviations.

3. We keep on doing this until there are no more returns left above or below the 3 standard deviation limits.

This way we obtain three different series, the first one with the up jumps, the second one with the down jumps, and the third the filtered returns.

Parametrizing the jumps

The outcome of the filtering iteration reveals that there are a total of 43 up jumps and 51 down jumps. These results allow us to obtain the frequency and distribution of the up and down jump functions.

The up jumps' expected frequency is 43 jumps every 3304 days -i.e. a frequency of 1.3014%. The down jumps' expected frequency is 51 jumps every 3304 days - i.e. a frequency of 1.5435%. The overall frequency is 94 jumps every 3304 days -that is, a frequency of 2.845%.

In order to characterize the exponential distribution function, the data gathered from both the sample of up jumps and the sample of down jumps are introduced into an optimization program, which estimates through the maximum verisimilitude method using the Chi Squared Test the parameters of the exponential distributions.

The output from the program is the mean of the exponential distribution \overline{x} ; to calculate its parameter λ , we thus need to apply the formula of the exponential distribution's mean:

$$\overline{x} = \frac{1}{\lambda} \Longrightarrow \lambda = \frac{1}{\overline{x}}$$
(1.20)

In the case of up jumps, the exponential distribution is on Table 3:



Table 3. Jumps Up adjusted Exponential Distribution

Evidences a 0.0422 shift of the function to the right, since this is the size of the minimum jump. Therefore, we

have to add this figure to the mean, which then becomes: mean = 0.01614 + 0.0422 = 0.05834. The variance obtained is: variance = 0.00026107.



 Table 4. Jumps Down adjusted Exponential Distribution

In the case of down jumps, we cannot generate an exponential distribution, as returns are now negative. We therefore need to convert the negative return distribution into a positive one in order to derive our distribution. When using it for the simulation, we thus turn to negative the result for the down jumps yielded by the distribution obtained. The actual result for the down jumps is shown.

The distribution derived from the optimization process is described on Table 4.

Having a mean = -0.018128 - 0.042294 = -0.06042, and variance = 0.00032861. Graphically, the adjusted curve is in the Chart 8.

Simulating the mean reversion motion with jumps

We use the above-stated formulas (1.13) and (1.14) to simulate the mean reversion process with the preceding parameters



Chart 3. Graphical output of the simulation of the mean reversion with exponential jumps model with 10,000 steps corresponding to 40 years.

The MATLAB code needed to simulate the process is set out in the appendix as MATLAB Code 1.

Conclusions

The model laid out above allows us to derive the parameters directly from market data, and makes it possible to adjust them according to executives' expectations. All parameters used in the model can be directly and intuitively understood, and its comprehension requires just average mathematical and statistical know-how.

The model is capable of coherently replicating the shifts in commodity markets, allowing for situations such as the one we have analyzed here, which involves a jump up in prices, to fit in.

The process of feeding and updating the model with new market data is simple and can be implemented both on MATLAB-type programs and on simulation-based spreadsheet programs.

APPENDIX

MATLAB Code 1

T=10000; %Number of periods
dt=1; %Time interval
N=T/dt;
Speed=.000452; %Reversion Speed
Sigma=.0125236; %Volatility of the process
paths=10; %Number of paths
S0=142; %Initial Value
S = 129.68; %Expected mean value
LambdaU = 0.013014; %Jump up frequency
LambdaD = 0.015435; %Jump down frequency
Lambda = 0.02845; %Total jump frequency
MeanPhiU = 0.016148; %Mean jump up
ShiftPhiU = 0.042288; %Jump up scaling
VarPhiU = 0.00026107; %Jump up variance
MeanPhiD = -0.018128; %Mean jump down
ShiftPhiD = -0.042294; %Jump down scaling
VarPhiD = 0.00032861; %Jump down variance
MeanPhi = MeanPhiU + ShiftPhiU + MeanPhiD + ShiftPhiD; %Mean of Phi
VarPhi = VarPhiU + VarPhiD; %Variance of Phi
<pre>UniformU = find(unifrnd(0,1,N,paths)>LambdaU);</pre>
UniformD = find(unifrnd(0,1,N,paths)>LambdaD);
dQUp = exprnd(MeanPhiU, N,paths) + ShiftPhiU;
dQUp(UniformU) = 0;
dQDown = -exprnd(-MeanPhiD, N,paths)+ ShiftPhiD;
dQDown(UniformD) = 0;
dQ = dQUp + dQDown;
Wiener=randn(N,paths);
SpeedDt=Speed*dt;
<pre>St=S0*ones(N,paths);</pre>
G1=exp(-SpeedDt);
G2=log(S+Lambda*MeanPhi*Speed)*(1-exp(-SpeedDt));
G3=Sigma*sqrt((1-exp(-2*SpeedDt))/(2*Speed));
G4=(1-exp(-2*SpeedDt))*(((Sigma^2)+Lambda*VarPhi)/(4*Speed));
for i=1:N
for j=1:paths
<pre>St(i+1,j) = exp(log(St(i,j))*G1+G2+dQ(i,j)+G3*Wiener(i,j)-G4);</pre>
end

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DIFFERENT RISK-ADJUSTED FUND PERFORMANCE MEASURES: A COMPARISON

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KEYWORDS

Value-at-risk, Extreme Value Theory, Mutual Fund Performance

ABSTRACT

Traditional risk-adjusted performance measures, such as the Sharpe ratio, the Treynor index or Jensen's alpha, based on the mean-variance framework, are widely used to rank mutual funds. However, performance measures that consider risk by taking into account only losses, such as Value-at-Risk (VaR), would be more appropriate. Standard VaR assumes that returns are normally distributed, though they usually present skewness and kurtosis. In this paper we compare these different measures of risk: traditional ones vs. ones that take into account fat tails and asymmetry, such as those based on the Cornish-Fisher expansion and on the extreme value theory. Moreover, we construct a performance index similar to the Sharpe ratio using these VaR-based risk measures. We then use these measures to compare the rating of a set of mutual funds, assessing the different measures' usefulness under the Basel II risk management framework.

INTRODUCTION

Evaluation of mutual fund performance is a key issue in an industry that has been rapidly evolving over the last few years; however, there is no general agreement about which measure is best for comparing funds' performance. Traditional fund performance measures are the ones developed by Sharpe (Sharpe 1966), Treynor (Treynor 1966) or Jensen (Jensen 1968) that use the mean-variance approach using the standard framework described in Markowitz (Markowitz 1952), namely using variance and covariance in the form of sigma or beta. However, another popular way to measure risk is the Value-at-Risk defined as the maximum loss corresponding to a given probability over a given horizon. Traditional VaR calculations assume that returns follow a normal distribution (Jorion, 2001), however, Favre and Galeano (Favre and Galeano 2002) introduced the modified VaR, which adjusts risk, taking into account skewness and kurtosis using the

Cornish-Fisher expansion (Cornish-Fisher 1937). Another approach would be to model only the tail of the distribution, in order to precisely predict an extreme loss in the portfolio's value. Extreme value theory (EVT) provides a formal framework to study the tail behavior of the distributions. The use of EVT for risk management has been proposed in McNeil (McNeil 1998), Embrechts (Embrechts 2000) and Gupta and Liang (Gupta and Liang 2005), among others.

In this paper we evaluate traditional risk-adjusted measures that are based on the mean-variance approach like with others that use VaR to quantify risk exposure, empirically testing the appropriateness of each within a sample of UK mutual funds.

The novelty of this paper lies in the use of the VaR calculation of losses using EVT and applying it as a risk measure to construct a performance index similar to the Sharpe ratio. Using EVT allows for a better estimation of the distribution of extremes and, consequently, provides a better estimation of the risk associated with a portfolio. We will also compare the rating of mutual funds using the different risk-adjusted performance measures.

This paper is organized in five sections. Section 2 reviews the different classical performance measures used in the analysis and introduces the modifications to obtain more accurate estimations. In section 3 we present the data and the sample statistics. Empirical analysis is presented in section 4 as well as differences in funds' ranking. The final section provides a brief summary and some concluding remarks.

PERFORMANCE MEASURES

Performance measures are used to compare a fund's performance, providing investors with useful information about managers' ability. We divide risk-adjusted performance measures into two types: traditional performance measures, based on the mean-variance approach, and VaR-based measures.

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) Traditional mutual fund performance measures are the Sharpe ratio, the Treynor index and the Jensen's alpha. The aim of the Sharpe ratio is to measure risk-adjusted performance of a portfolio. It quantifies the reward per unit of total risk:

$$S_i = \frac{R_i - R_f}{\sigma_i} \,, \tag{1}$$

where R_i represents the return on a fund, R_f is the risk-free rate and σ_i is the standard deviation of the fund. Treynor index measures the return earned in excess of a riskless investment per unit of market risk assumed.

$$T_i = \frac{R_i - R_f}{\beta_i} \,, \tag{2}$$

where R_i represents the return on a fund, R_f is the risk-free rate and β_i is the beta of the fund. Finally, Jensen's alpha measures the performance of a fund compared with the actual returns over the period. The required return of a fund at a given level of risk β_i can be calculated as:

$$R_i = R_f + \beta_i (R_m - R_f), \qquad (3)$$

where R_m is the average market return during the given period. The alpha can be calculated by subtracting the required return from the fund's actual return.

Nonetheless, there are other ways to measure risk. One of the most popular is Value-at-Risk (VaR). Value at Risk is defined as the expected maximum loss over a chosen time horizon within a given confidence interval, that is:

$$P(loss > VaR) \le 1 - \alpha , \tag{4}$$

where α is the confidence level, typically .95 and .99. Formally, Value-at-Risk is a quantile of the probability distribution F_X , or the *x* corresponding to a given value of $0 < \alpha = F_X(x) < 1$, which means

$$VaR_{\alpha}(X) = F^{-1}(x), \tag{5}$$

where F_{χ}^{-1} denotes the inverse function of F_{χ} .

We present four different approaches to VaR: normal VaR, historical VaR, modified VaR and extreme value VaR. Normal VaR assumes that the portfolio's rate of return is normally distributed. Historical VaR uses historical returns to calculate VaR using order statistics. Let $R^{(1)} \ge R^{(2)} \ge \cdots \ge R^{(T)}$ be the order statistics of the T returns, where losses are positive; then the $VaR_{\alpha}(R) = R^{(T\alpha)}$. The modified VaR takes into account not only first and second moments but also third and fourth ones. It uses the Cornish-Fisher expansion (Cornish-Fisher 1937) to compute Value-at-Risk analytically. And finally, extreme Value VaR uses Generalized Pareto Distribution (GPD) to obtain VaR. The upper tail of F(x) may be estimated by:

$$\hat{F}(x) = 1 - \frac{N_u}{n} \left(1 + \hat{\xi} \frac{x - u}{\hat{\sigma}} \right)^{-1/\hat{\xi}} \quad \text{for all } x > u \qquad (11)$$

To obtain the VaR_{α} we invert (11), which yields

$$VaR_{\alpha} = u + \frac{\hat{\sigma}}{\hat{\xi}} \left[\left(\frac{n}{N_u} (1 - \alpha) \right)^{-\hat{\xi}} - 1 \right], \quad (12)$$

where u is the threshold, $\hat{\xi}$, $\hat{\mu}$ and $\hat{\sigma}$ are the estimated shape, location and scale parameters, *n* is the total number of observations and N_u the number of observations over the threshold.

DATA

Our data set comprises monthly returns on 239 UK mutual funds over 11 years, from January 1995 to December 2005. The data were provided by Morningstar. Owing to the construction of the data set, we use only the data for funds that are active for the entire period. All mutual funds are measured gross of taxes, with dividends and capital gains, but net of fees. To illustrate the different methodologies and for the shake of simplicity, we have chosen the highest ten and lowest ten monthly averages return for the whole period. Table 1 summarizes detailed statistics of those funds.

Table 1: Descriptive statistics of the top ten and bottom ten average return funds.

Panel A: Bottom 10 funds							
Mean	Std.	Max.	Min.	Sk.	Ku.		
-0.002	6.672	14.934	-21.498	-0.236	-0.136		
0.050	6.632	17.934	-18.002	0.032	0.103		
0.080	5.636	13.712	-11.713	-0.019	-0.567		
0.127	5.633	13.778	-11.638	0.002	-0.548		

0.146	6.651	19.202	-15.840	0.297	-0.198
0.147	6.378	18.895	-20.506	-0.132	0.335
0.171	7.713	26.480	-21.025	0.143	0.531
0.212	6.234	26.352	-20.446	0.579	4.066
0.216	6.754	16.394	-13.878	0.244	-0.498
0.244	6.931	19.498	-15.877	0.345	-0.244
		Panel B: To	op 10 funds		
Mean	Std.	Max.	Min.	Sk.	Ku.
1.319	5.058	12.182	-14.900	-0.390	0.231
1.331	6.670	29.765	-21.934	-0.049	3.103
1.414	4.959	15.328	-14.597	-0.252	0.500
1.470	4.671	13.823	-10.472	-0.170	0.285
1.526	5.033	15.327	-13.883	-0.231	0.270
1.605	4.611	10.282	-16.008	-0.966	1.623
1.632	4.898	16.023	-17.239	-0.570	1.922
1.697	8.399	24.776	-18.913	0.282	0.740
1.771	6.453	27.880	-12.853	0.665	1.454
3.499	17.921	60.549	-70.528	-0.130	1.929

Mean=sample mean; Std. = Standard deviation; Max.=maximum observed monthly return; Min.= minimum observed monthly return; Sk.= Skewness; Ku. = Kurtosis

An examination of Table 1 shows that several funds have an asymmetric distribution. Upper fund returns have mostly negative skewness, indicating that the asymmetric tail extends toward negative values more than toward positive ones; however bottom fund returns show more negative skewness. According to the sample kurtosis estimates, the top ten fund returns show a higher level of kurtosis than the bottom ones. Table 1 also shows the highest and lowest month return for each fund: the highest one-month return is 60.5%, while the highest loss corresponds to the same fund (79.5%). These results indicate that some funds do not follow a normal distribution.

EMPIRICAL RESULTS

In this section we report and discuss results of the different performance measures. Table 3 shows the results of the classical performance measures: Sharpe, Jensen and Treynor, as well as the ranking of the fund that would result from those indexes. As expected, the bottom ten has a smaller index than the top ten. Moreover, for the bottom ten we have negative Sharpe and Treynor indexes and Jensen's alpha, meaning that those funds are not able to beat the market.

	Panel A: Bottom 10 funds							Panel B: 7	Гор 10 ft	inds	
Sharpe	Rank	Jensen	Rank	Treynor	Rank	Sharpe	Rank	Jensen	Rank	Treynor	Rank
-0.025	10	-0.372	10	-0.234	10	0.228	7	1.014	9	2.346	7
-0.017	9	-0.311	9	-0.169	9	0.175	10	0.959	10	1.602	10
-0.015	8	-0.075	3	2.371	1	0.252	5	1.119	8	2.724	2
-0.007	7	0.008	1	0.237	2	0.279	3	1.165	7	2.656	3
-0.003	6	-0.166	6	-0.039	8	0.270	4	1.229	6	2.944	1
-0.003	5	-0.221	8	-0.027	7	0.312	1	1.278	4	2.530	4
0.001	4	-0.191	7	0.007	6	0.299	2	1.298	3	2.475	5
0.007	3	-0.078	4	0.105	4	0.182	9	1.267	5	1.648	9
0.008	2	-0.091	5	0.101	5	0.249	6	1.414	2	2.386	6
0.011	1	-0.075	2	0.145	3	0.186	8	2.910	1	2.236	8

Table 3: Classical mutual fund performance measures

The other performance indexes are based on VaR. We have estimated $VaR_{0.05}$ and $VaR_{0.01}$ using the four different approaches discussed in section 2. To offer EVT VaR results we proceed with the generalized Pareto distribution (GPD) estimation. A crucial step in estimating the parameters of the distribution is the

determination of the threshold value. We have selected the proper threshold, fitting the GPD over a range of thresholds looking at what level ξ and σ remain constant. Because of space constraints and for the ease

of exposition, we do not present a detailed parameter estimation.

 $VaR_{0.05}$ and $VaR_{0.01}$ estimates are shown in Table 4. As expected, results for normal VaR and Cornish-Fisher VaR are similar for funds with little asymmetry and kurtosis. EVT VaR tends to be higher than the other

VaR thresholds when the return distribution is not normal and presents asymmetries and kurtosis, which is more frequent in the top group. Additionally, the bottom 10 funds have, in general, higher VaR values than the top ones, which means they are more susceptible to extreme events.

	Panel A: Bottom 10 funds								
	Va	R _{0.05}			Va	R _{0.01}			
Norm-VaR	Hist-VaR	Mod-VaR	EVT-VaR.	Norm-VaR	Hist-VaR	Mod-VaR	EVT-VaR		
10.977	10.289	11.449	13.697	15.524	15.259	16.608	18.641		
10.858	11.237	10.784	13.193	15.378	14.085	15.384	16.626		
9.190	9.531	9.286	10.481	13.031	11.412	12.365	11.572		
9.138	9.442	9.197	10.295	12.977	11.317	12.246	11.542		
10.794	9.956	10.270	12.231	15.326	11.796	13.787	14.650		
10.344	9.967	10.542	12.896	14.690	14.894	15.849	17.793		
12.516	11.522	12.122	14.638	17.772	19.225	17.976	20.182		
10.043	10.870	8.544	12.685	14.292	13.872	18.350	19.652		
10.893	10.107	10.501	11.636	15.496	13.081	13.650	13.437		
11.158	10.321	10.527	12.599	15.881	11.837	14.037	14.932		
			Panel B: T	op 10 funds					
	Va	R _{0.05}			Va	R _{0.01}			
Norm-VaR	Hist-VaR	Mod-VaR	EVT-VaR	Norm-VaR	Hist-VaR	Mod-VaR	EVT-VaR		

10.448

14.186

10.123

9.397

10.183

9.121

9.763

17.842

13.242

12.814

17.759

10.121

9.862

10.121

13.062

12.029

17.991

11.567

12.460

19.269

11.740

10.344

11.458

15.765

14.613

17.804

13.354

15.452

21.918

13.567

10.320

13.031

22.774

21.464

21.459

12.715

Table 4: VaR	results	of the	different	approaches
	results	or the	annerent	upprouenes

25.978	22.294	25.948	34.442	38.191	36.590	48.099	53.696
Norm-VaR:	normal-VaR; Hist	-VaR: Historica	l-VaR; Mod-V	aR: modified V	aR using Corr	ish-Fisher expa	nsion; EVT-
VaR: extrem	e-value-VaR calcu	ulated form the	GPD estimatio	n.			

9.846

14.439

10.248

9.228

10.283

10.774

11.375

15.303

10.002

With regard to performance measures and rankings, Table 5 shows the results of the modified Sharpe ratio using the $VaR_{0.05}$ in Table 4. The rank from each ratio is also in the table. The bottom group exhibits a very small ratio, and they show similar ranking regardless of the

7.098

9.927

7.242

7.252

7.192

6.669

5.800

13.104

8.103

7.552

9.315

7.054

6.415

7.061

7.175

7.058

11.332

7.489

7.001

9.641

6.743

6.213 6.753

5.979

6.425

12.118

8.844

method used for calculation. However, the results of the top group show more differences. To find out if they really produce similar results, we compared the rank order correlations of the top ten funds. Table 6 shows the Spearman and Kendall rank correlation.

Fable 5: VaR-based	performance	measures
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Panel A: Bottom 10 funds							
Norm-VaR	Rank	Hist-VaR	Rank	Mod-VaR	Rank	EVT-VaR	Rank
-0.015	10	-0.016	10	-0.015	10	-0.012	10
-0.011	9	-0.010	9	-0.011	9	-0.009	9
-0.009	8	-0.009	8	-0.009	8	-0.008	8
-0.004	7	-0.004	7	-0.004	7	-0.004	7
-0.002	6	-0.002	6	-0.002	6	-0.002	6
-0.002	5	-0.002	5	-0.002	5	-0.001	5
0.000	4	0.000	4	0.000	4	0.000	4

0.005	3	0.004	3	0.005	2	0.004	3
0.005	2	0.005	2	0.005	3	0.004	2
0.007	1	0.008	1	0.007	1	0.006	1
		I	Panel B: 7	Top 10 funds			
Norm-VaR	Rank	Hist-VaR	Rank	Mod-VaR	Rank	EVT-VaR	Rank
0.165	7	0.163	7	0.153	7	0.117	7
0.121	10	0.117	9	0.125	10	0.081	10
0.185	5	0.172	6	0.177	6	0.122	6
0.210	3	0.180	5	0.203	3	0.141	2
0.201	4	0.189	4	0.193	5	0.132	4
0.241	1	0.216	2	0.201	4	0.134	3
0.228	2	0.253	1	0.208	2	0.129	5
0.126	9	0.117	10	0.135	8	0.100	8
0.181	6	0.198	3	0.214	1	0.160	1
0.128	8	0.150	8	0.128	9	0.097	9

Not surprisingly, the Sharpe and the various VaR ratios exhibit higher correlations than do the Jensen and Treynor ratios. This is not unexpected, since Jensen and Treynor calculations include only the systematic component of risk, while the other measures also include residual risk. The normal VaR measure and the Sharpe ratio rate the ten top funds in the same order.

Table 6: Spearman and Kendall correlation of the performance measures for the top 10 funds

	Sharpe	Jensen	Treynor	Norm-VaR	Hist-VaR	Mod-VaR	EVT-VaR
Sharpe	1	0.248	0.782	1.000	0.891	0.770	0.745
Jensen	0.2	1	-0.006	0.248	0.394	0.394	0.297
Treynor	0.644	-0.067	1	0.782	0.636	0.588	0.673
Norm-VaR	1.000	0.200	0.644	1	0.891	0.770	0.745
Hist-VaR	0.733	0.378	0.467	0.733	1	0.879	0.782
Mod-VaR	0.644	0.378	0.378	0.644	0.733	1	0.927
EVT-VaR	0.600	0.244	0.511	0.600	0.600	0.867	1

Statistics in the top half of the matrix represent Spearman rank correlation coefficients; numbers in the lowest half correspond to Kendall values.

The modified VaR and EVT VaR also show a high correlation. With respect to the Kendall correlation, which is easier to interpret, the value of 0.867 indicates that there is an 87.6 percent greater chance that any pair will be ranked similarly than differently. Consequently, the chance of disagreement in the ranking between modified VaR and EVT VaR is 6.6%; however, the chance between the Sharpe ratio and EVT VaR is 20%.

Taking into account that only modified VaR and EVT VaR ratios allow asymmetry and kurtosis, the results of those measures would be more accurate in the calculation of performance measures for funds with non-normal returns. As a preliminary conclusion, these findings indicate that the comparison between Gaussian funds and non-normal ones is better done using those measures, since they are better able to capture the risk behavior among them.

Our sample data do not show a high degree of asymmetry, and so the Sharpe and normal VaR ratios

are highly correlated. In other words, risk measured through variance and the 0.95 quantile loss leads to the same ranking of performance measures.

CONCLUSIONS

We studied monthly returns of UK mutual funds, and we selected for the study the ten funds with the lowest and highest monthly average returns. For the distribution of the bottom ten, we reject that they follow normal distribution in all but one case. On the other hand, the upper ten show a higher degree of asymmetry and kurtosis, and we can reject normality in half of the cases. Also, we have calculated VaR using four different approaches, and EVT VaR is the one that gives higher results for probabilities of 0.05 and 0.01.

Regarding the ranking of performance measures, from the bottom sample we obtained the same ranking regardless of the measure used, except for the Jensen and Treynor measures, which also show a high rank correlation. However, for the top data set, the ranking is not the same. If we consider rankings from the modified Sharpe index calculated with the Cornish-Fisher VaR and EVT-VaR, more accurate measures in the presence of non-normal distribution, both are highly correlated and present a lower correlation with the other measures. So we recommend employing when trying to rank the performance of different funds, especially in the presence of non-normal data, such as returns from hedge funds or more frequently sampled returns.

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A MODEL FOR THE CREATION OF KNOWLEDGE AND COMPETITIVE SUSTAINABLE ADVANTAGES IN THE SUPPLY CHAIN

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Efficient consumer response, logistic operators, structural equations model, SEM.

ABSTRACT

This paper presents a model to measure the knowledge and sustainable competitive advantages generated by logistic operators, within the Efficient Consumer Response (ECR) framework. We present a definition of ECR practices, propose a model to measure the effects of these practices on final firm's results and develop a validation of the methodology, meeting the demands of related companies and logistic operators. The paper is part of a more general study trying to test the model on three groups of partners: firms operating with ECR practices, business consultants and researchers. The previous results allow us to conclude that logistic operators perceive these practices as relevant ones. The best valued items by the logistic operators are: human capital, improvement on individual labor and group climate, and improvement in learning and training firms plan.

INTRODUCTION

ECR is a joint strategy of suppliers and distributors to offer consumers highest value, best service and greatest variety of products; outcome of the collaboration on supply chain improvement and demand generation (Ferrer & Del Castillo (1996), Stern, El-Ansary & Hayes (1998), Whipple, Frankel and Anselmi (1999) AECOC, PROMARCA, 2000). A number of authors have stressed several necessary elements for ECR practices implementation success: key is the relationship amongst manufacturers and distributors (Merrefield, 1993), that demands changes in the firm's structure and processes (Shulman, 1993) and investment on information technologies. ECR processes must not be implemented distant from the creativity in merchandising and the firm's promotional activity (Veiders, 1993). ECR practices are strongly applied in the grocery industry, executive Information Systems

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(EIS), Electronic Data Interchange (EDI) and Radio derived devices (Buddembaum, 1994). Efficiency, flexibility and customer orientation are the main principles that manage the joint action of all the members in the supply chain in other to achieve the intended objective (Mejías, García, Prado, 2001). The adoption of practices in the ECR initiatives can introduce a change in various organization activities. Amposen (1991), Davenport (1998), Nonaka (2000), Ciborra and Andreu (2001) and Prusak (2002), amongst others, explain the change and learning experiences through the knowledge generation and management. To measure the ECR initiative impact on sustainable competitive advantages generation, we have drawn on the Technology Strategic Generic Actions (ITSGA) Information methodology (Andreu, Ricart and Valor, 1997). Other authors have recently paid attention to this methodology: to incorporate into the firm's strategic objectives the experiences of other firms and the possibilities offered by information and communication technologies, to achieve competitive advantages (Palou, 2006), on strategic planning (Holistic consulting), for value chain redesign by paying special attention to the synergies amongst different processes (Soto and Tapia, 2006) and in the planning strategy derived from information technologies and information systems (IT/IS) (Gil and Guarch, 2006).

THE MODEL: OBJECTIVE AND HYPOTHESES

In this study we propose a model for the measure of knowledge and competitive advantages generation in the "Efficient Consumer response practices" (ECR) area. This implies the identification, selection, and validation of intellectual capital and its competitive advantages indexes (that we have named "associated concepts"), the study of enablers and promoters in the implementation and the revealing of critical success factors. The measurement model is composed of two blocks: knowledge and competitive advantages. We have revisited the ongoing models, see references, and the Intelect Euroforum model has been the basis of our analysis. It is easy to understand and according to

Bueno, Rodríguez and Salmador (2003): open, flexible and universal. Many important firms in Spain have applied this model (among others PriceWaterhouse Coopers, Telefonica R+D, Inditex Group and the Public Administration). To measure the impact of the ECR practices in sustainable competitive advantages (SCA) we made use of the methodology for strategic planning ITSGA. It tries to identify "strategic generic actions" that can promote sustainable competitive advantages. Firms as Sears, Federal Express or TRW have identified a group of ITSGA categories for strategic applications as e.g.: transactions with customers, new products development and establishment of a group of collaboration agreements. Besides, some authors as de Pablos et al. (2006) and consultants' groups have considered and applied this methodology for standard actions identification. Combining the mentioned tools, we propose our model for the intellectual capital measurement composed of three parts: human capital (HC), structural capital (SC) and relational capital (RC). To measure the sustainable competitive advantages (SCA) we propose 5 categories: "product", "customers", "channels", "providers" and "general". By analogy, we name the second SCA block ECRSGA (strategic generic actions based on ECR practices). Each of these 8 blocks (3 of Intellectual Capital (IC) and 5 of ECRSGA) is divided into 41 elements, items in the survey. That will help us to validate the model. At the same time, each item presents a group of non exclusive alternative answers. All this means 176 variables, measured via "perceptions of improvement" based on a Likert scale.



Figure 1 - Model for IC, SCA in the ECR practices measurement (Soret, 2007)

According to the literature review (see introduction), we have selected a group of variables to include in the model; allowing us to measure the impact of ERP initiatives in final firm's results.

Model variables. Source: Intelec Model (Bueno et al.
2003)
Human capital measurement
Improvement of individual and work conditions
Managerial style
Learning improvement
Education-training
Organizational environment
Integration of people in the firm
Promotion, rewards
Structural capital measurement
Data mining techniques
Procedures manual
Improvement of processes
Communities of practices
Relational capital measurement
Customer standards
Customer satisfaction
Loyalty programs
CRP, CPFR techniques
ASN techniques

Sustainable Competitive Advantages measurement Source: Andreu et al. (1997), Andreu and Sieber (2000) Improvement of information to SC and consumers Improvement of the communication offered to the SC Degree of personalization of the product to providers Information on new products Innovation and price to final customers



This way, considering the eight defined blocks, we propose the following hypotheses:

H01	ECR initiative generates and/or increases firm's
	the human capital
H02	ECR initiative generates and/or increases firm's
	relational capital
H03	ECR initiative generates and/or increases firm's
	structural capital
H04	Knowledge reached by the adoption of ECR
	practices generates sustainable competitive
	advantages related with the product
H05	Knowledge reached by the adoption of ECR
	practices generates sustainable competitive
	advantages related with the product
H06	Knowledge reached by the adoption of ECR
	practices generates sustainable competitive
	advantages related with the distribution channels
H07	Knowledge reached by the adoption of ECR

	practices generates sustainable competitive advantages related with the providers
H08	Knowledge reached by the adoption of ECR practices generates sustainable competitive advantages related with the firm's general aspects

Figure 3 : Hypotheses

The three (basic) first hypotheses are part of the general hypothesis (theoretical hypothesis): the ECR initiative generates or increases the human, structural and relational capitals. Increasing, therefore, the firms' intellectual capital. The same way, the rest of the "basic" hypotheses are part of another "theoretical" general: the knowledge generated by adoption of ECR practices generates sustainable competitive advantages, related with a group of categories. To sum up, we are trying using a confirmatory analysis, to find out if the generation and/or increase of intellectual capital promotes sustainable competitive advantages in the ECR initiative.

The 176 variables and indexes for the perception increase are divided into nine different blocks: block I is composed by human capital indexes, block II by structural capital indexes, block III by relational capital indexes, from block IV up to block VIII, different indexes for sustainable competitive advantages are shown. Block IX refers to the study of what we have named "associated concepts", as enablers in the implementation and critical success factors and is not part of the former confirmatory analysis.

THE ANALYSIS METHODOLOGY

In order to obtain information, 15 interviews were carried on with experts in a group of firmsⁱ that operate ECR initiatives. Amongst them, we formed an eight experts panel. By group dynamics work, and a previous deep interview with each member, we agreed on the main structure for the general model. With the help of another panel of experts in market research, we elaborated the final questionnaire. For obtaining the data from the sample, and on an attempt to increase the number of respondents, we organized a professional seminar in ESIC (Business and Marketing School), Madrid, with researchers of the Rey Juan Carlos University and the collaboration of LOGICA, the Spanish organization grouping logistic operators. The seminar call was announced as follows: in the economic press during 4 days, an e-mail was sent to 2.500 potential participants, information on radio during a whole week and in the web page www.eriete.com. From the seminar, we got 65 completed surveys. After that we still got 27 via personal interview. The data have been processed using SPSS and AMOS.

The factorial analysis reveals some dimensions for the different blocks in the model that will be used as measurable variables in a model of structural equations, SEM, containing latent variables and measurement

errors. The general model for the structural equations systems is a formal mathematical model, a group of linear equations that include variables that can be directly observed and measured and latent variables that represent concepts that cannot be directly observed. Our model of measurement for IC and SCA adapts perfectly to the structure of a lineal structural equations model. Composed by two sub-models: the structural model, that relates among them the latent variables(HC, SC, RC and SCA); and the measurement model, that relates each latent variable with the variables measuring it in a direct way (the indexes). The model establishes that there is a direct relationship of the three capitals with the SCA generation and a certain relationship amongst those capitals. Besides, the measurement errors are explicitly included for each variable in the process of estimation. To check the results we carried out a Bayesian

estimation The sample was generated, 10 complete groups of data, by the Markov Chain Monte Carlo method, MCMC, with a diffuse distribution as *a priori*. This way, we were able to obtain a sample of 900 data, enough for the estimation.

MAIN RESULTS

The variables have been grouped into 28 factors: 8 for HC, 4 for SC, 10 for RC and 6 for SCA. Each dimension groups various elements in the obtained factor structure. These dimensions or factors will be the used as measurable variables in the model of structural linear equations.

We have obtained a global satisfactory adjustment of the structural equation model. The results for each latent variable with their factors, the regression standardized weights and their correspondent p-values, are presented in figure 4.

HUMAN CAPITAL	(Estimation, p)
Improvement of individual and wo conditions	rk(0'654, 0'000)
Managerial style	(0'596, 0'000)
Learning improvement	(0'465, 0'000)
Education-training	(0'415, 0'000)
Organisational environment	(0'158, 0'000)
Integration of people in the firm	(-0'233, 0'000)
Promotion, Rewards	
STRUCTURAL CAPITAL	
Data mining	(0'545, 0'000)
Procedures manual	(0'200, 0'000)
Improvement of processes	(0'065, 0'049)
Communities of practice	(-0'269, 0'000)
and virtual university	

RELATIONAL CAPITAL	(Estimation,p)
Customer standards	(0'862, 0'000)
Customers satisfaction	(0'182, 0'000)
GXC	(0'100, 0'002)
Loyalty programs	(-0'272,0'000)
CRP, CPFR ASN	(-0'155,0'000)
SUSTAINABLE COMPETITIVE AD	VANTAGES
Improvement of information to SC and consumers	(0'725, 0'000)
Improvement of communication to SC	(0'224, 0'000)
Personalisation of the product to	(0'134, 0'000)
Information on new products	(-0'214.0'000)
Innovation and price to final customers	(-0'179,0'000)

Figure 4 - Standard weights of the model variables and p-value

In relation with the previous results and with the group of basic hypotheses 1,2 and 3 -those relating to the adoption of practices in the ECR initiative, the generation or increase of the human, structural and relational capital in the organisations- there exists a direct relationship amongst the following variables: individual improvement and work conditions, managerial style, improvement of learning skills, training, the management by objectives and the work environment. All have a direct impact in the increase of HC.

The increase of SC can be obtained by the adoption of data mining techniques, generation of manuals establishing procedures and continuous process improvement.

The increase of RC is directly related with the creation and/or improvement of the standards for customers, their satisfaction, and the management by categories and the loyalty programmes.

Concerning to the group of basic hypotheses 4 to 7 -that is with firms that relate the increase of intellectual capital with the generation of sustainable competitive advantages (SCA)- there is a direct relationship amongst the following variables: the improvement of information to the supply chain and to the consumer, the improvement of the communication to the supply chain and the personalisation of the product to providers.

The theoretical hypothesis 1 and 2 have been verified. This means that ECR is a technique for individual and organisational learning, and the creation of knowledge and this generates sustainable competitive advantages for firms and organisations in the area of efficient consumer response, ECR. Or, in other words, ECR improves the organisational results by the creation of SCA.

			Estimation	Р
Structural Capital	<	Human Capital	,024	***
Relational Capital	<	Human Capital	-,332	***
Relational Capital	<	Structural Capital	3,336	***
Competitive Advantages	<	Human Capital	,041	,009
Competitive Advantages	<	Relational Capital	,184	***
Competitive Advantages	<	Structural Capital	,582	,002
FACTOR1CE	<	Structural Capital	1,000	
FACTOR2CE	<	Structural Capital	-,990	***
FACTOR3CE	<	Structural Capital	3,155	***
FACTOR4CE	<	Structural Capital	,352	,049
FACTOR8CH	<	Human Capital	-,051	,016
FACTOR7CH	<	Human Capital	,447	***
FACTOR6CH	<	Human Capital	-,041	,071
FACTOR5CH	<	Human Capital	,118	***
FACTOR4CH	<	Human Capital	,184	***
FACTOR3CH	<	Human Capital	-,111	***
FACTOR2CH	<	Human Capital	,515	***
FACTOR1CH	<	Human Capital	1,000	
FACTOR8CR	<	Relational Capital	,016	,460
FACTOR7CR	<	Relational Capital	-,150	***
FACTOR6CR	<	Relational Capital	-,002	,948
FACTOR5CR	<	Relational Capital	-,007	,834
FACTOR4CR	<	Relational Capital	,100	***
FACTOR3CR	<	Relational Capital	-,259	***
FACTOR2CR	<	Relational Capital	1,000	
FACTOR1CR	<	Relational Capital	-,099	***
FACTOR1VCS	<	Competitive Advantages	1,000	
FACTOR2VCS	<	Competitive Advantages	-,272	***
FACTOR3VCS	<	Competitive	,109	***

			Estimation	Р
		Advantages		
FACTOR4VCS	<	Competitive Advantages	-,256	***
FACTOR5VCS	<	Competitive Advantages	,111	***
FACTOR9CR	<	Relational Capital	-,033	,158
FACTOR10CR	<	Relational Capital	,085	,002
FACTOR6VCS	<	Competitive Advantages	,132	***

Figure 5 - Structural equations model

We present some conclusions derived form the global adjustment of the structural equations model

CONCLUSIONS

The results seem quite interesting ones. All the coefficients that interconnect the variables of interest, the different capitals considered and the sustainable competitive advantages are positive and besides with p-values lower than 0,001.

For the human capital the highest valued items by the logistic operators are: the improvement in the individual and group labor climate (FAC3 2 = 31,631) and the improvement in learning (FAC4 $\overline{3}=31,874$) and training classes in the named "associates concepts". For the structural capital, the improvement in the process efficiency, the improvement in the customer systems (Data Warehouse) and the improvement in organizational systems. For the relational capital, the participation in ECR practices in general and in CRP, KFA, DRO (continuous replenishment, key file alignments, delivery and reception orders) in particular. For the sustainable competitive advantages: the communication agreements in the distribution, the personalization of the product and the improvement in the portfolio and promotions for customers.

The intellectual, human, structural and relational capitals have a direct and positive influence in generation of sustainable competitive advantage. We can also appreciate that there is a positive relationship amongst the different capitals considered: in the structural capital, the biggest impact on the increase is produced through the human capital and the relational capital increases, because the human and structural capitals. It seems that the generation of knowledge can provide to firms the achievement of sustainable competitive advantages.

The previous results in the structural equation model, joint to the descriptive analysis, allow us to conclude that, probably and in a significant way, the logistic operators perceive some practices as relevant ones. The best valued items by the logistic operators are: human capital, improvement in the individual labor and group climate, improvement in the learning and training classes in the "associated concepts". By focusing in the structural capital, the most important relationships are in the improvement in the efficiency in processes, the improvement in systems to improve the relationship with customers (Data warehouse) and the improvement in organizational systems. For the relational capital, the participation in ECR practices in general and in CRP, KFA, DRO (continuous replenishment, key file alignments, delivery and reception orders) in particular. For the sustainable competitive advantages part: the communication agreements in the distribution, the product personalization and the improvement in the portfolio and customer promotions.

However, we think it is important to go deeper in the factors that do not allow a satisfactory fit for the particular case of the logistic operators. That it is the reason why, we must wait for further conclusions until our research allow us to obtain better results. Amongst the most important barriers we have found in our analysis, we have to stress the size of the sample used. The structural equations models requires of a wider sample. We have tried to solve this problem by applying the Markov Chain Montecarlo methodology; apart from this, firms are quite reluctant to offer some data needed for the qualitative research. For these reasons, we suggest as future research to keep on developing deep interviews with the people responsible, in the firms, of the areas of our interest, so that this can offer us to clear son cause-effect relationships, and go deeper on the study of the best industry practices and, specially in the ones we have been unable to find a definitive conclusion.

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ⁱ The analysed firms show their desire for being not mentioned by considering of strategic importance the provided information



EUROPEAN REGIONAL POLICY: AN ASSESSMENT IN THE CONTEXT OF A GROWTH MODEL

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KEYWORDS

Public inputs, agglomeration, integration.

ABSTRACT

This paper analyzes, within a regional growth model, the impact of productive governmental policy and integration on the spatial distribution of economic activity. Integration is understood as enhancing territorial cooperation between the regions, and it describes the extent to which one region may benefit from the other region's public input, e.g. the extent to which regional road networks are connected. Both integration and the characteristics of the public input crucially affect whether agglomeration arises and if so to which extent economic activity is concentrated: As a consequence of enhanced integration, agglomeration is less likely to arise and concentration will be lower. Relative congestion reinforces agglomeration, thereby increasing equilibrium concentration. Due to the congestion externalities, the market outcome ends up in suboptimally high concentration.

INTRODUCTION

Supporting convergence and intensifying European territorial cooperation are among the key objectives of European regional policy for the period of 2007-2013. One of the instruments to reach these goals is the further improvement of the transport infrastructure which is funded from structural and cohesion funds. Considering whether such an instrument is apt to reach the goal of convergence is part of both theoretical and empirical analysis. Aschauer (1989) provided a seminal work in which he derives a strong positive relationship between infrastructure and growth. This could basically speed up convergence. However, more recent contributions in the macroeconomic literature find more modest returns to infrastructure investment (see e. g. Gramlich (1994) for an overview). Within endogenous growth theory, those models strongly influenced by Barro (1990) analyze fiscal policies if a productive governmental input serves as a growth determinant. These models have been continuously refined to allow for different characteristics, especially congestion, of the public input (see e. g. Glomm and Ravikumar (1994a, 1994b) or Turnovsky (2000) for an overview): However, all these considerations focus on the view of a single country and, if they analyze convergence at all, they view it as the process leading to an equilibrium growth path. Consequently it is not possible to explain the distribution of economic activity across space as a mere consequence of interacting regions.

This concern lies at the heart of models known as 'new economic geography' (see Krugman (1995)). These models single out imperfect competition, increasing returns and transportation costs as fundamental resources shaping the economic landscape, but few focus on governmental activity. An exception is the work of Martin and Rogers (1995): They focus on the role of infrastructure as facilitating transactions, i. e. the trade within and between countries. Consequently agglomeration is reinforced as result of governmental activity. Puga (2002) analyzes the impact of regional policy expenditures on mitigating regional disparities and highlights that a undifferentiated consideration of infrastructure neglects that different characteristics of infrastructure also operate differently. Consequently, a thorough analysis of the impact of regional productive governmental policy also requires a sophisticated modelling of the public input.

However, though all these new economic geography

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models include regional governmental policies, they exclusively consider infrastructure in reference to reduced transportation costs; by contrast, the Barro type models assume a productive governmental input but neglect regional interaction. The European Union primarily regards infrastructure as production input that enhances the productivity of the other local inputs. Consequently, viewing infrastructure as reducing transportation costs is too narrow if one wishes to analyze whether the newly intended European regional policy will be successful in reducing regional disparities.

These shortcomings of the existing literature are the starting point for this model: We analyze the impact of regional policy on agglomeration. In doing so, regional policy thereby includes the provision of infrastructure that basically may be interpreted in a broad sense as comprising any facility, good or institution provided by the government that enhances the productivity of the other private inputs. This allows for a consideration of physical infrastructure such as roads, airports, telecommunication networks, but also basic research and training networks of education infrastructure. These different types formally may be represented by integrating a congestion function adopted from Eicher and Turnovsky (2000) which includes relative and absolute congestion as well as capital spillovers. We use this modelling of the governmental input and implement it in a modified version of the regional growth model of Bröcker (2003), who for his part focuses on learning-by-doing and interregional knowledge diffusion.

Integration between the two regions is modelled as the extent to which one region may benefit from the other region's public input. With this formulation we rely on Alesina and Spolaore (2003, chapter 6) and are broader than the usual approach of the new economic geography which assumes that integration predominantly reduces transport costs and thereby strengthens agglomeration. Our setting is in line with the goal of the European regional policy mentioned before, namely of enhancing European territorial cooperation. Integration may be also achieved, for example, by increasing the flow of ideas between regions as already argued by Rivera-Batiz and Romer (1991) and others. We assume identical production technologies with constant returns to the private inputs for the two regions. Labor is immobile while capital accumulation is taking place in the region with the higher productivity. The resulting equilibrium is based on equalized productivities of capital, and it determines the equilibrium capital distribution. Depending upon the interaction between agglomeration and dispersion forces, multiple equilibria with different stability characteristics may arise. It is shown that the bifurcation point is a function of congestion, capital spillovers and integration. The endowment with immobile labor acts as threshold value that determines which equilibrium capital distribution finally results. Agglomerations reflect equilibrium capital distributions with different regional capital stocks. In analogy to Krugman (1991), the region displaying the bigger capital stock may then be interpreted as being the core, while the other region is the periphery.

In the light of this model, convergence in the sense of the European Union may be interpreted as a reduction in concentration. Basically this may be derived by integration or by the type of the governmental input provided, i. e. the choice about the degrees of congestion and spillovers. The following relationships become evident from numerical simulations: Integration reduces concentration since it allows the periphery to access the core's public input and hence to benefit from its productivity. In contrast to this, relative congestion is associated with a negative capital externality and aggravates concentration. As a consequence, the resulting market equilibrium ends up in suboptimally high concentration. The impact of capital spillovers may be ambiguous: Basically agglomeration forces are strengthened by capital spillovers since the productivity advantage of the core gains importance. Nevertheless, strong spillovers may smooth concentration if combined with a high degree of relative congestion. This is the consequence of decreasing marginal returns in the governmental input.

THE ANALYTICAL FRAMEWORK

Firms in both regions i = 1, 2 produce the homogenous good, Y_i , by the same Cobb-Douglas technology. The inputs used in each region are immobile labor, L_i , and private capital, K_i . We eliminate mobile labor from the analysis, because it essentially follows the distribution of capital. Furthermore, output depends upon regional access to a global public input that is measured by an index, D_i . The production function for a representative firm in region i is given by

$$Y_l = L_l^{\lambda} K_l^{\alpha} D_l^{\gamma}, \quad \lambda > 0, \quad 1 > \alpha > 0, \quad 1 > \gamma > 0 \quad (1)$$

The global public input, D_i , includes the regional public inputs, G_{si} , that are separately provided by both regions. The firm's access to the other region's public input may be limited as parameterized by $0 < \beta < 1$, and we assume

$$D_1 = G_{s1} + \beta G_{s2} \tag{2a}$$

$$D_2 = G_{s2} + \beta G_{s1} \tag{2b}$$

Correspondingly, the parameter β may be interpreted as a measure for the extent of integration between the two regions: If $\beta = 0$, firms in each region only benefit from the public input provided by their local governments, and consequently the scope of governmental policy is restricted to their own region. In contrast to this, $\beta > 0$ implies that firms in one region also have (at least partial) access to the other region's public input. What we have in mind is the following: If the government of a certain region provides education for the early childhood, with the goal to increase the productivity in its own region, the impact on the other region's productivity probably will not be affected significantly (at least if labor is immobile). Formally, β will be close to zero. The same argument applies to the provision of a university that restricts the access to students stemming from its own region. If, in contrast to this, the government of region 1 provides universities which are open to students from region 2 (and if graduates return to their home region), productivity in both regions will increase as consequence of governmental activity in one single region. Then, β will be positive.

The modelling of the governmental input is adopted from Eicher and Turnovsky (2000), and the public input provided by the local government in region *i* may be characterized as follows

$$G_{sl} = G_l \left(\frac{K_l}{K_l}\right)^{\varepsilon_R} \overline{K}_l^{\varepsilon_A}, \quad 0 \le \varepsilon_R \le 1, \quad -\alpha \le \varepsilon_A \le 1 \quad (3)$$

Thereby $\overline{K_i}$ denotes the aggregate stock of private capital in region *i*, and G_i denotes the aggregate flow of government expenditure. Function (3) incorporates the potential for the public good to be associated with alternative types and degrees of scale effects or congestion as denoted by ε_A and ε_R . In contrast to Eicher and Turnovsky (2000), we do not restrict the sign of ε_A to be negative, but we allow for positive and negative externalities at the aggregate level. Note that the integration parameter β is also a measure for the extent to which the arising externalities of one region have a bearing on the other region. Above, the actual level of ε_A is of major importance for the resulting equilibria.

BALANCED STEADY STATES

The equilibrium is based on equalized productivities of private capital. Individuals in the two regions are able to hold capital in region 1 or in region 2. Physical capital is only mobile as long as it is not yet nailed down. Hence, the adjustment process of marginal capital returns takes time.

Denote the ratio of marginal capital productivities with

$$R \equiv \frac{\partial Y_1}{\partial K_1} / \frac{\partial Y_2}{\partial K_2} \tag{4}$$

A balanced steady state is characterized by a stationary capital distribution, i. e. by R = 1. In case of initial productivity disparities (i. e. $R \neq 1$), the prevailing capital ratio is not stationary; but over time transitions to a steady state with k increasing (if R > 1) or decreasing (if R < 1) will take place. Hence an equilibrium is only attained after a certain transition period, but k converges to a stable equilibrium in finite time. Since we assumed that capital is immobile once it has been nailed down, a transition with increasing k implies that during the transition period there is only investment in region 1 and no

investment in region 2. The capital stock in region 2 then declines with the depreciation rate, δ .

DETERMINANTS OF AGGLOMERATION: CORE AND PERIPHERY

Note that since we focus on a growing economy, we assume that the governments in both regions set the aggregate expenditure levels, G_i , as a constant fraction, θ_i , of aggregate capital, $\overline{K_i}$,

$$G_l = \theta_l K_l, \quad 0 < \theta_l < 1 \tag{5}$$

An expansion in government expenditure is then parameterized by an increase in the capital share, θ_i . Additionally we have to take into account that in equilibrium $\overline{K_i} = N_i K_i$ applies. Then

$$\tilde{g}_s = \theta k^{1 + \varepsilon_A} n^{1 + \varepsilon_A - \varepsilon_R} \tag{6}$$

defines the equilibrium ratio of governmental activity, and $\theta \equiv \theta_1/\theta_2$.

In equilibrium the ratio of marginal capital productivities turns out to equal

$$R = l^{\lambda} k^{\alpha - 1} \left(\frac{\tilde{g}_s + \beta}{1 + \beta \tilde{g}_s} \right)^{\gamma - 1} \cdot \left(\frac{\alpha(\tilde{g}_s + \beta) + \gamma \varepsilon_R \tilde{g}_s}{\alpha(1 + \beta \tilde{g}_s) + \gamma \varepsilon_R} \right)$$
(7)

Taking logarithms, after some simple manipulations, yields

$$R \ge 1 \iff i(k) \ge -\lambda \ln l$$
 (8)

with

$$i(k) \equiv (\alpha - 1) \ln k + (\gamma - 1) \ln \left(\frac{\tilde{g}_s + \beta}{1 + \beta \tilde{g}_s}\right) + \ln \left(\frac{\alpha(\tilde{g}_s + \beta) + \gamma \varepsilon_R \tilde{g}_s}{\alpha(1 + \beta \tilde{g}_s) + \gamma \varepsilon_R}\right)$$
(9)

Depending on the characteristics of i(k) it is possible to attain either one unique equilibrium or multiple equilibria, the latter showing different stability characteristics.

Formally, the underlying equilibrium is unstable whenever function i(k) is positively sloped in the equilibrium capital. If then, starting from the steady state capital ratio, the relative capital productivity in region 1 increases (R > 1), the resulting capital productivity advantage in region 1 attracts investment and induces further increases of k. Hence the capital distribution departs continuously from the initial steady state and the system diverges from the unstable equilibrium. The argumentation holds analogously if, starting from an initially unstable equilibrium, the capital ratio is reduced and then declines continuously. If on the contrary the function i(k) is negatively sloped for equilibrium capital ratios, an increase in k reduces the ratio of capital productivities (R < 1), thus giving rise to a productivity advantage in region 2. Then k declines and converges again to its original steady state value.

Following Krugman (1991), the region which holds the higher capital stock then represents the core of the entire economy, whereas the other region is the periphery. The analysis will be carried out for equally distributed immobile labor, l = 1; hence the threshold value is given by $-\lambda \ln l = 0$. The argumentation focuses on those determinants that affect the run of function i(k) and the underlying economic effects will be discussed. Two aspects gain especial importance: the sign of i'(k), which determines whether agglomeration forces (i'(k) > 0) or dispersion forces (i'(k) < 0) prevail; and the multiplier that decides on the extent of the arising forces.

NUMERICAL SIMULATIONS

As argued before, agglomeration only occurs if regional spillovers are sufficiently high. Concerning this argument, the bifurcation point separates conditions in which one unique equilibrium arises from those that go along with multiple equilibria.

Nevertheless, higher values of ε_A do not automatically result in more concentration. The following calculations and simulations illustrate the sensitivity of the model with respect to those parameters that represent the externalities, ε_A and ε_R , as well as integration, β . We show their impact on the number of equilibria in the context of Table 1 and analyze their impact on concentration within Figures 1 and 2.

Table 1: Bifurcation points $\overline{\epsilon}_A(\beta, \epsilon_R)$

	$\varepsilon_R = 0.2$	$\varepsilon_R = 0.23$	$\varepsilon_R = 0.35$
$\beta = 0.2$	-0.7	-0.72	-0.76
$\beta = 0.25$	-0.1	-0.28	-0.5
$\beta = 0.3$	1.78	0.56	-0.22

Tables 1 and 2 show values of the threshold values $\overline{\epsilon}_A$. For scale effects which exceed this level, agglomeration takes place. The tables illustrate how the levels of the bifurcation points $\overline{\epsilon}_A$ are affected by integration and relative congestion. The gray values in Table 1 refer to the bifurcation points indicated in Figure 1, while the gray values in Table 2 correspond to Figure 2.

The tables could be interpreted as follows: Increasing integration unequivocally raises the value of the bifurcation point and thus supports the hypothesis that integration mitigates agglomeration forces. The contrary applies with respect to ε_R : There the level of the bifurcation point is reduced with increased congestion, and agglomeration becomes more likely.

Within the graphical simulations in Figures 1 and 2, we

Table 2: Bifurcation points $\overline{\varepsilon}_A(\beta, \varepsilon_R)$

	$\varepsilon_R = 0.4$	$\varepsilon_R = 0.5$	$\varepsilon_R = 0.6$
$\beta = 0.5$	0.9	0.29	0.06
$\beta = 0.6$	2.11	0.7	0.3
$\beta = 0.7$	5.22	1.26	0.58

analyze how ε_A , ε_R and β impact on concentration as measured by the equilibrium capital distribution, k^* . As far as possible, we assume symmetry, $\theta = n = l = 1$. Hence the threshold value $i^*(k) = 0$ is represented by the horizontal axis. We consider constant returns to scale in the private inputs ($\alpha + \lambda = 1$) and make sure that the condition of endogenous growth is fulfilled ($\alpha + \gamma(1 + \varepsilon_A) =$ 1). Under these conditions (at least) one equilibrium with equal distribution of capital, i. e. $k^* = 1$, results and no agglomeration takes place within it. If, instead, multiple equilibria arise, the region displaying the higher capital stock represents the core, whereas the other region may be interpreted as being the periphery. The equilibria are symmetric in the sense that one could easily change the region's indices and would have the same implications as before, but now from the point of view of the other region. Higher equilibrium values of k^* are interpreted as reflecting more concentration.

Figures 1(a)-1(c) plot the equilibrium capital distributions for alternative degrees of integration and assume intermediate relative congestion, $\varepsilon_R = 0.5$. The levels of the bifurcation points, $\overline{\epsilon}_A$, are indicated next to the respective degrees of integration. Solid lines represent high regional spillovers ($\varepsilon_A = 0.9$), while the dashed lines correspond to low levels ($\varepsilon_A = -0.2$). Since the simulations assume $\alpha = 0.3$, we choose this lower benchmark for ε_A to fulfill the condition $-\alpha < \varepsilon_A$. In case of $\varepsilon_A = -0.2 < \overline{\varepsilon}_A$, the prevailing agglomeration forces are too low, capital is equally distributed across the regions, and $k^* = 1$. If, instead, $\varepsilon_A = 0.9$, agglomeration is basically possible (see Figures 1(a) and 1(b)). But more integration reduces concentration (lower k^*) since then the smaller region may also benefit from the spillovers of the bigger region. Consequently, capital accumulation does not move to the core. Figure 1(c)displays a situation in which dispersion forces dominate in either case and $k^* = 1$. As argued before, increasing integration reduces the agglomeration forces.

Figures 2(a) – 2(c) emphasize the model's sensitivity and focus on alternative levels of relative congestion for $\beta = 0.25$. Again the levels of the bifurcation points are included in parenthesis below each figure. Solid and dashed lines reflect ε_A in analogy to Figure 1, and equal distribution only arises if $\varepsilon_A < \overline{\varepsilon}_A$. The dashed function in Figure 2(a) is one example. All other combinations of β and ε_R lead to agglomeration, and the following structure may be observed: Increasing relative congestion fosters agglomeration in either case. But note that



Figure 1: The impact of integration if $\varepsilon_R = 0.5$ parameters: $\alpha = 0.3 \ \lambda = 0.7, \ \theta = 1, \ n = 1, \ l = 1 \Rightarrow i^*$: horizontal axis

solid line: $\varepsilon_A = 0.9$, dashed line: $\varepsilon_A = -0.2$

concentration is even more pronounced for low levels of ε_A . The intuition for this result is as follows: On the one hand, we have intra-regional spillovers which foster concentration due to ε_A . But on the other hand, there are decreasing returns not only in private capital but also in the governmental input. With an increase in spillovers, ε_A , the ratio of individually available governmental inputs, \tilde{g}_s , increases; hence decreasing returns gain importance and reduce concentration. However, as the simulations illustrate, the total effect always implies agglomeration, not only for low but also for high values of relative congestion. Since there is a negative capital externality which goes along with congestion, individuals overestimate private capital return. Hence, agglomeration may even become more concentrated due to an increase in congestion. Nevertheless, the congestion externalities induce a suboptimally high level of concentration.

CONCLUSION

The basic objective of this paper is to analyze the impact of regional policy on the spatial distribution of economic activity. We ask whether integration will increase concentration as usually shown in new economic geography models which mostly interpret integration as a re-



Figure 2: The impact of relative congestion if $\beta = 0.25$ parameters: $\alpha = 0.3$, $\lambda = 0.7$, $\theta = 1$, n = 1, $l = 1 \Rightarrow i^*$: horizontal axis

solid line: $\varepsilon_A = 0.9$, dashed line: $\varepsilon_A = -0.2$

duction in transport costs. Additionally we ask whether the European regional policy to foster territorial cooperation will reach the goal to support convergence. Within the context of the model presented, regional policy includes the extent of inter-regional cooperation, as well as the type of the governmental input provided. This input affects output not only directly but also indirectly as it enhances the productivity of the other inputs. Since the governmental input is characterized by absolute and by relative congestion, the model may be adopted to a variety of interpretations; two examples are physical infrastructure or research networks. It is shown that either one unique or multiple equilibria arise, with the latter showing different stability characteristics. Whether or not this leads to convergence in the sense of the European Union's regional policy goals depends upon a variety of economic conditions.

The model is very sensitive to the assumed parameter constellations, but nevertheless some general results may be derived: Integration unequivocally reduces concentration since it allows the smaller regions access to the other regions' public input and hence to benefit from its productivity impact. This result stands in strong contrast to those analysis that model infrastructure as facilitating trade. Relative congestion is associated with a negative capital externality and aggravates concentration. As a consequence, the resulting market equilibrium ends up with suboptimally high concentration. This argument reflects the typical discussion within growth literature about the impact of relative congestion. The effect of intra-regional capital spillovers is more complex. Agglomeration only arises if spillovers are strong enough to overweigh decreasing returns to private capital. Nevertheless, if a high level of capital spillovers applies in a situation of high relative congestion, the impact may be reversed and decrease the resulting concentration.

The model's policy implications could then be summarized as follows: More integration reduces regional disparities, while relative congestion operates in the opposite direction. These congestion externalities could be internalized by a fiscal policy that corrects for the distortions. With this, it is clear that much work is still left to be done.

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TAYLOR-TYPE RULES AND PERMANENT SHIFTS IN PRODUCTIVITY GROWTH

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ABSTRACT

This paper uses simulation techniques to evaluate variants of the Taylor rule in a model where the underlying trend rate of growth is subject to permanent shifts. We show that the original Taylor rule is not particularly well-formulated for dealing with this type of environment. However, we also find that a Taylor-type rule in which the output gap is replaced by output growth or one that is augmented by an explicit policy response to deviations of the price level from a target path will look much like the optimal policy.

INTRODUCTION

During the 1970s, there was a worldwide slowdown in productivity growth accompanied by a rising inflation trend. In the 1990s, the opposite occurred—an unexpected rise in real growth was accompanied by a surprising decline in the inflation trend. In both episodes, the shift in real productivity growth appeared to be permanent. There is empirical evidence (Kiley 2003) that medium-to-low frequency measures of inflation and productivity growth are negatively correlated in U.S. data. He explains the regularity as an inherent dynamic of the New Keynesian Phillips Curve.

In this paper, we show that the negative correlation is driven by the monetary policy regime. In a New Keynesian model with sticky prices with optimal policy, there would be no correlation between these trends. The optimal policy is probably not feasible. However, we show that there are feasible policies that approximate the optimal policy and would greatly reduce or even reverse the sign of the correlation between these trends. This is true in a model with a New Keynesian Phillips Curve.

The Taylor rule (Taylor, 1993) was originally intended as a purely descriptive device—a way of characterizing what monetary policymakers tended

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to do in practice. Although not the optimal policy in any particular model, the Taylor rule has been shown to work well in a variety of models and in situations where the policymaker is uncertain about the trends and structure of the economy. However, one situation in which it does not work well is when there are permanent shocks to technology growth. In this paper, we use simulation techniques to show how the Taylor Rule fails to deliver good policy. We also show one might modify the Taylor rule in such an environment to improve policy.

The next section describes the model we use and motivates our interest in permanent technology growth shocks. Then, we use the model to explain the macroeconomic dynamics under optimal policy which provides a benchmark for evaluating practical policy options. We evaluate alternative policies that have been recommended to deal with transitory shocks to technology growth and show that they also work well in the presence of permanent shocks.

THE NEW KEYNESIAN MODEL

We modify a simple New Keynesian model used in earlier work (Gavin et al. 2005) to include shocks to the growth of the exogenous technology factor (Pakko 2002). The model features a welldefined demand for money, sticky prices, and a Taylor type interest rate rule for implementing monetary policy.

Households are infinitely lived agents who seek to maximize their expected utility from consumption, c_t and leisure, l_t ,

$$E_0\left[\sum_{t=0}^{\infty}\beta^t\left(ln(c_t)+\chi\frac{l_t^{1-\sigma_t}}{1-\sigma_1}\right)\right],$$

subject to the following budget constraint, time constraint, and capital accumulation equation:

$$P_{i}(c_{i} + i_{i}) + M_{i} + B_{i} =$$

$$P_{i}w_{i}n_{i} + P_{i}q_{i}k_{i} + D_{i} + M_{i-1} + R_{i-1}B_{i-1} + T_{i},$$

$$l_{i} + n_{i} + s_{i} = 1, \text{ and } k_{i+1} - k_{i} = \phi(i_{i}/k_{i})k_{i} - \delta k_{i},$$

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where B_t is government bonds, P_t is the price level, i_t is investment, M_t is the nominal money stock, w_t is the real wage rate, n_t is labor, q_t is the rental rate on capital, k_t is the capital stock, D_t is the firms' profits remitted to the households, R_t is the gross nominal interest rate, T_t is a transfer from the monetary authority, δ is the depreciation rate, and s_t represents the shopping-time costs of holding money balances $s_t = \zeta (P_{c_t} / M_t)^{\gamma}$. The parameter ϕ represents capital adjustment costs which are given by $i_t - \phi(i_t / k_t)k_t$. In the steady state $\phi(i_t / k_t) = i / k$ and $\phi'(i_t / k_t) = 1$.

In the steady state, labor is fixed as the technology factor and consumption growth at rate g. The household Euler equation is complicated by the presence of the shopping time specification. For the moment, consider a shopping time function that depends only on real balances and not on consumption. In such a case leisure will be separable in utility and we would have the standard intertemporal Euler equation associated with log utility.

$$\frac{c_{t}}{\beta c_{t+1}} = (1+r_{t}) \tag{1}$$

where r_t is the real interest rate on one-period bonds. In a stable, long-run equilibrium, consumption will grow at rate g. Equation (1) shows that the interest rate will be:

$$(1+r) = \frac{(1+g)}{\beta} \, .$$

That is, the real interest rate will be positively related to the underlying growth rate of the economy.

Firms produce heterogeneous goods which are aggregated into a composite consumption good. Sticky prices are generated by a standard Calvo pricing framework in which only a fraction of the firms are permitted to reset their prices each period.

The firms are monopolistically competitive producers of output, $y_{j,t}$, according to

$$y_{j,t} = (k_{j,t})^{\alpha} (Z_t n_{j,t})^{1-\alpha},$$

where *j* indicates the number of periods since the firm last adjusted its price, $n_{j,t}$ is firm labor demand, $k_{j,t}$ is firm demand for capital and Z_t is an economy wide productivity factor.

The most important extension of the model for this paper is a technology process by which the longrun growth trend is subject to variation over time. The technology shock in this case is a composite of a growth shock (Z_{gt}) and a level shock (Z_{lt}) : $\ln(Z_{t}) = \ln(Z_{gt}) + \ln(Z_{t})$, where each of these shocks follows an independent AR(1) process:

$$\ln(Z_{lt}) = \rho_{z} \ln(Z_{lt-1}) + (1 - \rho_{z})\overline{Z} + v_{lt}, \text{ and}$$

$$\ln(Z_{gt} / Z_{gt-1}) = \rho_{g} \ln(Z_{gt-1} / Z_{gt-2}) + (1 - \rho_{g}) \ln(\overline{g}) + v_{gt},$$

where \overline{g} is a trend rate of growth used as the baseline for model simulations. We consider a series of experiments using a special case for which the growth shocks are permanent; i.e., $\rho_g=1$. The level shocks are assumed to be highly persistent with $\rho_z=0.95$.

Each period, every firm must make two decisions. First, firms determine the cost minimizing combination of capital and labor given their output level, the wage rate, and the rental rate of capital services. Second, the pricing decisions are made. In particular, the probability a firm can set a new price is η and the probability a firm must charge the price that it last set *j* periods ago is $(1-\eta)$. The composition of output purchased by households is

$$y_t = \left[\sum_{j=0}^{\infty} \eta (1-\eta)^j y_{j,t}^{(\varepsilon-1)/\varepsilon}\right]^{\varepsilon/(\varepsilon-1)},$$

where $y_t = c_t + i_t$.

Before describing the policy rule, we briefly describe the assumptions used to assign values to the model parameters. In the utility function, the value of σ_1 is set at 7/9. The steady state labor share is 0.3. That calibration implies a labor supply elasticity of real wages approximately equal to 3. The household discount factor is 0.99. The shopping time parameter, γ , is set to unity, implying an interest rate elasticity of money demand equal to -0.5. The capital share of output is set to 0.3 and the capital stock is assumed to depreciate at 2 percent per quarter. The price elasticity of demand is set equal to 6, implying a steady state markup of 20%. We set the probability of price adjustment equal to 0.25 implying that firms change prices on average once a year. The average and marginal capital adjustment costs around the steady state are zero (i.e., $\varphi(\cdot) = i / k$ and $\varphi'(\cdot) = 1$). The elasticity of the investment-to-capital ratio with respect to Tobin's q, $\chi = [(i/k)\varphi''(\cdot)/\varphi'(\cdot)]^{-1}$, is set to 5.

The model is closed with a monetary policy rule. Taylor (1993) showed that the path of the federal funds rate during the period from 1987 through 1992 could be fairly well-described by a simple rule by which the nominal interest rate was manipulated in response to two gaps: the gap between observed inflation, π_t and the target rate, π^* , and gap between output, y_t , and its long-run equilibrium level, y^* . The Taylor rule can be written as:

$$R_{i}^{*} = \overline{r} + \pi_{t} + \theta_{\pi}(\pi_{i} - \pi_{i}^{*}) + \theta_{y}(y_{i} - y_{i}^{*}) + u_{i}.$$
(2)

In this specification, Taylor treated the real interest rate, \overline{r} , and the inflation target, π^* , as constants (both set equal to 2.0 in the original work). He set both reaction parameters, θ_{π} and θ_{y} , equal to 0.5. In our work we add a weakly persistent interest rate error (autocorrelation coefficient set to 0.3) written as $u_t = \rho_u u_{t-1} + \varepsilon_{ut}$. The inflation target also follows a persistent AR1 process with the autocorrelation coefficient set equal to 0.95 in our simulations: $\pi_t^* = \rho_{\pi} \pi_{t-1}^* + (1 - \rho_{\pi}) \overline{\pi} + \varepsilon_{\pi t}$.

We include two policy shocks because we think it is important to make a distinction between shocks to the central bank's long-run objective and shocks to the liquidity position (or the short term interest rate). Although the two are not independent in the long run—the long-run inflation rate must be consistent with the accumulation of short-run liquidity positions--there is no reason to think that these shocks will be correlated in the short run.

We develop a baseline policy, approximately optimal, with which to compare the Taylor and alternative rules. We say approximately because the distortions due to monopolistic competition and the shopping time friction are small relative to the distortion associated with sticky prices and, therefore, are ignored. Perfect inflation stabilization (an infinite value for θ_{π}) would eliminate the sticky price distortion. We approximate the optimal policy by setting $\theta_{\pi} = 9999$ and $\theta_{y} = 0$.

INTEREST RATE RULE DYNAMICS

Figure 1 shows the model response of inflation to a 0.1% shock to the quarterly growth rate of the technology factor—this results in a permanent increase in the long-run growth rate from 1.6% to 2.0% at an annual rate. The figures show percent deviations from steady state values for the optimal policy and the Taylor Rule regime. Under the optimal policy, the inflation rate is zero.



Figure 1: Inflation Response to Real Growth Shock

As we saw in Equation (1), the higher growth of consumption is associated with a higher real interest rate. Under the optimal policy, the central bank keeps inflation at the steady state target and the nominal interest rate rises to match the increase in the real rate. Under the Taylor Rule the increase in wealth leads to an increase in demand that is split between higher output and higher inflation. The fundamental flaw in the Taylor rule is that it depends in part on the steady state path for real output. When there is a permanent increase in the growth rate, there is an ever increasing rise in the perceived output gap (until the central bank can learn about the trend and adjust the parameters of the rule). The initial rise of inflation causes an increase in price dispersion among firms, markups fall, and output rises above the optimal path. Both the nominal and real rates rise above the optimal path. Households work and save too much under the Taylor Rule policy. The get the real rate higher, the inflation rate must rise. In this case, it rises in the first year and falls thereafter.

To see why inflation must eventually fall in the Taylor Rule case, note that by Equation (2) the deviation between the real rate from \overline{r} is equal to θ_{π} times the inflation gap plus θ_{y} times the output gap. Since the real rate remains above the optimal rate for an extended period, an ever growing output gap must be partially offset by a negative inflation gap. This problem does not occur in the flexible price model because the real rate does not have to rise above the optimal path. The flexible price outcome for real variables is essentially the same as in the optimal economy because there is no distortion associated with a dispersion of prices across firms.

The permanent growth shock is an increase in expected lifetime income for the household. Under the optimal policy, the increase in wealth leads people to consume more goods and more leisure immediately. Figure 2 shows the impulse responses of the capital stock to the same shock.



Figure 2. Capital Response to Real Growth Shock

Following the shock people want to smooth consumption of both goods and leisure. Under the optimal policy, with inflation steady, there is no distortion from sticky prices and output does not rise as it does with the Taylor Rule. The desire to work less leads to an initial decline in savings and investment. The capital stock falls below the steady state and does not return to the previous steady state path for about 5 years. Note that after 5 years, there will be a new steady state path for output and the capital stock.

The capital stock does not decline as much (almost not at all in this case) as in the optimal policy because the higher interest rates (and higher wages) encourage people to work more, supplying enough output to support a bit higher consumption and much more investment than in the optimal case.

Note also that we are conducting our experiments under the assumption that the central bank does not recognize the change in the growth rate of technology immediately. The steady state growth rate for all real variables will change. Intuitively, our investigation is to find policies that will work well while the central bank learns about these changes.

Alternative Policies

Even if the policymaker wanted to follow an optimal policy, conditions under which inflation variability can be literally reduced to zero are quite restrictive. It is unlikely that such a policy is feasible in practice. There are two important insights that suggest ways for policymakers to get closer to the optimal policy. The first was made by Athanasios Orphanides (Orphanides 2003) who specifically recommends using the growth rate of output rather than the output gap in the policy rule because there noise in estimates of potential output. We assume that the path of potential output is smooth so that changes in the output gap are dominated by changes in actual output. Therefore, not much is lost by responding to output growth rather than the output gap. Furthermore, given the appropriate choice of the reaction coefficient on output growth, the policy

can prevent any long-deviation of inflation from target because it allows the real rate to grow in proportion to the growth rate. In Equation (1), with log utility specification, the real rate rises one for one with the balanced growth rate. The first row of Table 1 shows the policy parameters we use to compute the impulse responses of inflation, the capital stock and the real interest rate under the output growth rule (labeled as Diff y in the charts).

The other insight (from Svensson 1999) is that when a central bank cannot commit to an inflation target, it can achieve the commitment outcome by adopting a target for a price level path. Essentially, this is the same as adopting a long-run or multi-period average inflation objective. The central bank must correct past deviations of inflation from target in order to stay on the path. This prevents the inflation from declining over time as we saw in the 1990s following the increase in productivity growth.

Our second rule is a rule for the price level path. We adopt the policy that we used in earlier work and was found to work well in reducing long-run inflation risk (Gavin et al. 2009). This rule reacts one for one to changes in inflation and also to deviations of the price level from a path for the price level that is growing at the target inflation rate. The rule is written as $R_{t}^{*} = \overline{r} + \pi_{t} + \theta_{n}(p_{t} - p_{t}^{*}).$ The parameters for this price level path rule are shown in the second line of Table 1.

Table 1. Policy Parameters

Diff y	$\theta_{\pi} = 0.5, \ \theta_{dy} = 1$
Price Path	$\theta_{\pi} = 0, \ \theta_p = 0.2$
Combination	$\theta_{\pi} = 0, \theta_{dy} = 1, \ \theta_p = 0.2$

The impulse responses of inflation and the capital stock for each rule are shown in Figures 3 and 4 with the optimal case.



Figure 3. Inflation Response to Growth Shock



Figure 4. Capital Response to Growth Shock

Figures 3 and 4 show that both policies look much more like the optimal policy than does the Taylor Rule. Including the price path in the rule allows some inflation following the growth shock, but it keeps longer-run expectations near the target. A key result, that both policies keep the real interest near the optimal path.

COMPUTATIONAL EXPERIMENTS

In this section we examine the performance of each of these rules as well as a combination rule when there is a larger mix of shocks disturbing the economy. The shocks are distributed normally with mean zero. The standard deviations (s.d.) of the shocks are scaled for quarter data. The shock to the technology level (s.d.=.0075) explains about 70 percent of the variance in output. The output growth shock (s.d.=.001) is calibrated to replicate the uncertainty in aggregate output and the variability induced by growth shocks reported by Gorodinchenko and Shapiro (2007). The inflation target shock (s.d. = .001) is calibrated to roughly match the range of desired inflation objectives that appear in Federal Reserve official testimony and speeches. The liquidity shock is calibrated to approximately match the error that is induced by the use of 25 basis point discrete changes in the fed funds target. As a consequence, even at the (approximately) optimal policy, there will still be some inflation volatility due to policy shocks.

We examine four policies: the Taylor Rule, the output growth rule, the price path rule, and a combination rule that includes the reaction to output growth in the price path rule. See the bottom line of Table 1 for the parameters in the combination rule.

In each experiment, we simulate two models—the one with the optimal policy response and one of four alternative policies. In each of 10,000 iterations, we start at the steady state and generate 40 quarters of data using random generated innovations for each of the shocks. Then we report the root mean squared deviation of inflation and output growth in the alternative policy case from the optimal policy outcome. The results for inflation and output for the Taylor Rule and our

three alternative policies are shown in Figures 5 and 6, respectively.



Figure 5. Long-Run Uncertainty about Inflation



Figure 6. Long-Run Uncertainty in Output Growth

In Figure 7, we show the correlations between inflation and output growth over different time horizons. At one quarter, average inflation and output growth are positively correlated for all four policy regimes. Over horizons longer than one year, the trends are positively correlated for all regimes, except for the Taylor Rule.



Figure 7. Correlations over Different Frequencies

CONCLUSION

This paper shows that the Taylor Rule performs poorly in the presence of permanent output growth shocks. However, policies that have been suggested to deal with temporary growth shocks also work well in the presence of permanent shocks. The negative correlation between inflation and productivity growth may be explained by monetary policy that pays too much attention to the output gap.

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TOWARDS AN OPTIMAL SYNTHETIC INDEX FOR MEASURING GENDER INEQUALITY

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KEYWORDS

Synthetic indicators, Gender, Inequality, Modelling.

ABSTRACT

Gender equality is a key aspect of human rights in order to achieve sustainability and development focused on people. Bearing in mind how important equality has become in decision making, indicators including the gender approach are useful for quantifying the differences between the two genders and how they have evolved over time.

Taking gender into account brings a diverse and complex reality into play which, in order to analyse accurately, entails distinguishing between various approaches and technical alternatives. This paper presents modelling, understood as creating a simplified recreation of a complex reality, as the most suitable framework.

A thorough analysis of recent literature reveals serious limitations, thus leading to the need to further research in areas such as the adaptation of empirical indicators to the theoretical framework, the expression applied when calculating simple indicators, the process used when rescaling them for normalisation purposes, the average used to obtain a synthetic index and the methods used to assign weights to integrated simple indicators. We have focused our research on these aspects, analysing and contrasting different alternatives, particularly focusing on ascertaining the most accurate methodology to attain a synthetic gender indicator, as a way of analysing these phenomena.

INTRODUCTION

Analysing gender equality is a very relevant subject in human development. In this sense, the Platform for Action of the IV World Conference on Women, which took place in Beijing in 1995, assigns a strategic objective to the need to gather and disseminate information broken down by gender and specific to the realities of women. In addition, it is worth highlighting that the third of the Millennium Development Goals (MDG), an international agreement signed by 189 countries in September 2000 and seconded by the United Nations, is "to promote gender equality and empower women". Consequently, tools to measure

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) José María Riobóo University of Santiago de Compostela Department of Quantitative Methods El Burgo s/n. 15782 Santiago, Spain E-mail: josem.rioboo@usc.es

gender are essential, implying indicators that focus particularly on analysing the relative position of men and women.

This is the specific function of gender indicators as well as to detect the social changes both genders experience at different moments in time. More specifically, the use of synthetic indices involves aggregating several partial indices in order to carry out more aggregated analyses. In the process of obtaining them, there are very many occasions in which the researcher has to adopt resolutions, implying choosing from several suitable alternatives. In this sense, the simulation and development of alternative scenarios will allow us to obtain optimal results.

Having specified the target, we need to accurately establish the variables to be considered in accordance with their importance and data availability. The fact that various techniques and models can be used to select variables allows us to determine alternative scenarios, which at the same time are open to analysis, in order to establish a final set of variables.

In a second stage, criteria are defined to group the selected variables in order to determine the strata on which to obtain the synthetic indicators. The variety of options available when grouping demands the application of several techniques and models in order to determine the most suitable strata in terms of number and composition.

Prior to obtaining these indices, different alternatives are required for the variables under consideration and they must be measured in equivalent terms. This in turn requires research into various rescaling methods and their implications.

Finally, the paper discusses the application of the extensive and diverse Theory of Index Numbers to the topic this paper is concerned with. Aggregation, averaging and weighting methods provide us with a complex scenario for which various research alternatives are available and where the optimality sought after will depend on the properties previously deemed desirable for the indices to be obtained.

This paper is structured as follows: Firstly, we present the aims of this research. Next, we make reference to the statistical sources that we have used and list them by topic. The next section details the methodology used to obtain simple gender indicators for all the variables considered. We then analyse several rescaling alternatives for these indices, following which we compare the different methods to obtain the synthetic indices of gender equality through the aggregation of partial indices that integrate the areas considered. In the next section results are presented along with the most significant conclusions drawn. The last section includes a series of bibliographical references in the field of gender indicators.

OBJECTIVE

The general objective of this research is to obtain indicators that facilitate the incorporation of the gender approach in the production of statistics as an important aspect of including gender equality issues. We therefore aim to further the research into determining a suitable methodology for obtaining a system of gender indicators that provides us with a real picture of each gender's roles, structures and needs, as well as verifying the compliance and effects of the agreements signed and activities undertaken respectively on a regional, national and international scale to foster equality.

INFORMATION SOURCES AND VARIABLES

The methodological contributions this paper makes are also applied in an empirical analysis of data referring to Spain. In order to do so, various official statistical sources are used that allowed us to periodically access reliable information broken down by gender. This information is essential for establishing the proportion of men and women in each of the different socioeconomic categories. The main shortcoming in this sense is that this breakdown usually appears for macro type data, which implies that we are missing information as we go deeper into more specific levels or when data gets mixed up with other variables.

This research takes into account annual data on 36 variables broken down by gender between 2000-2007. In order to obtain objective gender indicators, this selection, following criteria based on data availability, reliability and significance, only includes variables that are clear "positive" or "negative" in terms of gender equality. Hence, the most confusing, such as demography, nationality, religion, etc, have been excluded. However, it must be said that for comparative purposes, this set of variables is expressed in relative terms.

Once selected, the variables are grouped by dimensions of social concern, determined according to classifications of the situation of men and women used by international organisations, such as the United Nations (Gender Statistics Base) and the Organisation for Economic Co-operation and Development (Gender, Institutions and Development Database): Power and decision making, Social assistance, Education, Activity and Healthcare.

PARTIAL GENDER INDICATORS

The choice of partial indicators depends on the preestablished goal of constructing a synthetic index, and implies multiple criteria based on a general consensus regarding the suitability of a set of desirable characteristics that these indicators should have. These characteristics cover aspects as: *suitability*, that is, the degree to which the indicators fit the theoretical reality they are representing: *accessibility*, how readily available they are; *comprehensibility* or how easy they are to interpret; and *comparability* in terms of both time and space.

Indicators of gender equality, which are based on the existence of a gender role, aim to establish the relative situation of men and women and the changes that have occurred at different moments in time. The idea is to measure aspects linked to equality and inequality of gender, where such aspects can be measured, quantified and systemised. Therefore, gender indicators are tools used to understand social processes and provide informed and equitable options to maximise the positive impact of an intervention in this direction.

As there is such a wide variety of indicators, researchers must choose the most relevant and those which can be measured, always bearing in mind their ability to be compared to indicators elaborated in other fields and over time, whereby chronological series make it possible to study variable trends over time. Likewise, researchers should choose the indicators that are most common and easily transferrable from one type of action to another.

However, prior to this we must choose the type of variable to be used, that is, whether to employ levels, variations or growth rates, to name a few, as well as the type of data, that is, the original series, the cycle trend or the seasonally adjusted series, etc.

This paper aims to compare the indicators most commonly used to analyse gender equality, from which we have chosen the two below due to they are relative indicators, omitting absolute indicators which limit our analysis due to not providing points of reference:

$$G1_i = \frac{W_i}{M_i} * 100 \tag{1}$$

$$G2_i = \frac{W_i}{T_i} * 100 \tag{2}$$

where we calculate, for the *ith* observation, the percentage that represents the variable of our study

referring to women (W_t) over men (M_t) and over the total of both genders (T_t) , respectively. We should mention here that the G2 index is also known as the feminisation index.

We explain both partial indices in the same way. In both cases gender equality would occur when the indicator scores 100, but if the value is below this figure, women would be in inferiority in relative terms, which could be either positive or negative depending on the connotations of variable in question.

NORMALISATION OF PARTIAL INDICATORS

The procedure used to build synthetic indicators for each of the dimensions considered comes from normalising simple indices obtained from the variables of each area. In this way we can eliminate the distorted effects of different scales (Mardia et al. 1979). There are several ways that enable us to normalise these indices (Freudenber 2003; Jacobs et al. 2004) when confronting the normalisation of scale values and the possibility of biases. The main methods to obtain these standard variables, \tilde{X}_{y} , that is to say, variables in a common scale, are as follows:

1. Standardisation:

$$\widetilde{X}_{ij} = \frac{X_{ij} - \overline{X}_{j}}{\sigma_{i}}$$
(3)

where *p* is the number for simple indicators $I_{l,I_2,...,I_p}$ with values for a set of *n* observations; X_{ij} is the value of the *ith* observation for *jth* indicator, with $1 \le i \le n$ y $1 \le j$ $\le p$; being \overline{X}_j the arithmetic average for the *jth* indicator and σ_i its standard deviation.

2. Ratio or percentage differences from the mean:

$$\widetilde{X}_{ij} = \frac{X_{ij}}{\overline{X}_j} \tag{4}$$

3. Ratio or percentage differences over periods:

$$\widetilde{X}_{ij} = \frac{X_{ij}^{t} - X_{ij}^{t-h}}{X_{ij}^{t-h}}$$
(5)

4. Lineal rescaling techniques, highlighted among them:

a)Minimal rescaling:

$$\widetilde{X}_{ij} = \frac{X_{ij} - X_{\bullet j}}{X_j^{\bullet} - X_{\bullet j}} * 10$$
(6)

where $X_{\bullet j}$ is the worst value according to the *jth* indicator and X_{j}^{\bullet} is the best one.

b) Maximal rescaling:

$$\widetilde{X}_{ij} = \frac{X_j^{\bullet} - X_{ij}}{X_j^{\bullet} - X_{\bullet j}} * 10$$
(7)

Our work focuses on comparative results obtained from applying the standardisation and minimal rescaling methods, as they are the predominant alternatives at present.

When this point is reached, it is important to clarify the best and worst values of the indicator, references necessary to carry out minimal rescaling (Drewnowski 1972). The definition of these values is based on the definition of the synthetic index we are aiming to calculate. As this research aims to find an indicator to measure how the discrimination of women has evolved, the positive or negative connotation of each variable must be taken into account in order to discern the values that represent a better situation for women. Therefore, if the variable has positive connotations, the higher the value of the indicator the better and the less discrimination, whereas if the variable has negative connotations, the higher the indicator the higher the level of discrimination of women is.

Matters could be made easier by considering only the variables that associate high simple index values to more positive circumstances for women, that is, less discrimination, rather than those that are associated to lower values, but this is not the case in this research. Another alternative to simplify the method above would be to change the sign of simple indices values belong to variables with negative connotations. As per Hair et al. (1999), this inverse scoring method is more suitable when a factorial analysis is to be undertaken as it avoids the possible effects of variables offsetting one another when we really should consider that they both point in the same direction when it comes to the final objective being measured. This paper adopts this procedure and, as a result we do not need to identify the highest and lowest values scored by women for each and every variable. In all cases, the best score will be the highest value of the index and vice-versa.

Bearing these considerations in mind, the normalised index will make it possible to analyse the evolution of gender equality over time, assigning a value of 10 when the situation for women was at its best and 0 should the opposite apply.

If we opt for standardisation as a method to calculate normalised variables we turn simple indicators into a standard scale with a zero average and standard deviation one, which also allow us to add them up properly (World Economic Forum 1996). In this case, the interpretation of standardised simple indices would be the same as that for minimal rescaling, the higher the indicator the better the circumstances are for women. The greatest drawback of this method would be in the cases where data distribution is not centred around its mean, because the presence of outliers will affect results substantially (McGranahan et al. 1972). Nevertheless, this drawback may be overcome by applying detection outlier techniques or also by applying winsorized and trimmed means.

It is worth highlighting that unlike simple indicators, which captured differences between genders, both normalised and standardised indicators and also the synthetic indicators calculated using them as a basis, will only provide information about the evolution of the discrimination of women.

Although the normalisation methods mentioned above are the usual practice, we believe future research should test alternative methods of short-term stable normalisation to overcome the shortcoming of periodical redefinition.

SYNTHETIC INDICATORS

Once we have established a partial indicator system, that is to say, the set of the integrated and systematic indices related to gender equality that allow us to quantify the variety of aspects this topic involves, a synthetic index must be obtained for each dimension along with a final synthetic index. In order to do so, we need to make decisions over the two of the most relevant aspects: how to determine the weights and averages we are going to use.

Determining weights

In the process used to add up simple indices, we need to address the subject of weighting, due to the fact that one of them might have different significance in the aggregated index. The systems used the most to assign weights could be divided into four groups:

-- Factorial Methods, Principal Component Analysis being the most popular. Used by several authors to set up indicators (Ram 1982 and Slotje et al. 1991, amongst others), this method aims to explain most of the total variability in a set of variables using the least possible number of components, defining these as a new category of independent variables that are lineal functions of the original ones. When applying this method we are able to consider the normalised partial indices through the factorial charges in the first principal component.

-- Equal or unitary weights. Using standardised variation rates as partial indices allow for symmetrical treatment as a result of the equal variance inherent to standardisation. This method can be considered suitable in the case of working with dimensions of equal size. The primary shortcoming of this method is that the choice of partial indicators must be highly filtered due to the sensitivity of results to any deviation.

-- Use of quantifiable reference variables. In this case, weights can be determined on the basis of the relevancy of the indices according to each magnitude. We can distinguish three different alternatives: a) based on the involvement of each partial index in the aggregate of reference, b) based on the simple or partial correlation between partial indices and reference variable, c) based on the results of a model of lineal programming, such as DEA (Data Envelopment Analysis) initially proposed by Charnes, Cooper and Rhodes (1978) and applied by Zhu (2001) to establish weights when finding synthetic indices.

-- Qualitative weights. In this scenario weights are assigned according to subjective criteria resulting from the knowledge of the phenomenon we are considering. The most commonly used subjective criterion assigns weights according to the degree in which they comply with the most desirable theoretical properties for the different indices mentioned above.

This classification does not include all the methods available for assigning weights, as specific and sometimes complementary alternatives exist, such as the use of "Budget Allocation" (Winterfeld 1986) and the "Hierarchy Process" (Saaty 1987).

Given that in general terms the choice of weighting system has an important impact on the value of the indicator, in our analysis diverse alternative models have been tested, focusing mainly on the first two criteria mentioned: Principal Component Analysis and equal weighting.

Aggregating partial indicators

Once the measurement units of the elementary indices are homogenised, we proceed to aggregate them in order to obtain the synthetic index. In order to do so, two groups of techniques are often used: additive and multiplicative techniques, depending on whether the index is obtained from operations derived from aggregating the different elementary indices (ex.: arithmetic average) or if it is obtained from operations derived from their product (ex.: geometric average).

When determining the most suitable aggregation procedure, we must bear in mind the characteristics of both the elementary indices to be grouped and also their units of measurement, such as the average and weights to be used. Any error in this sense could lead synthetic indices to be biased, in that they would not correctly reflect the basic information. It has been demonstrated that the so called "scale effect", "average effect" and "weighting effect" interact when determining the value of the synthetic index, being able to go so far as to be compensating or to impel the index value in the wrong direction. Under a scales criterion, we group the aggregation methods in three key blocks: 1. When we work with ordinal scales the aggregation can be obtained simply by summing up the ranges. 2. If the considered scale is an ordinal one, we can obtain the aggregation as the difference between the number of indicators that are over and under the average or an arbitrary deviation according to it. 3. If we have a ratio scale, as is often the case in this kind of studies, aggregation implies that we have to determine the average we are going to use, as well as the weights, bearing in mind all the implications derived from the previous normalisation process.

For the average of relative magnitudes (percentages, rates, indices, etc.) there is sufficient justification from a theoretical point of view that the geometric average is the most suitable. However, in practice the arithmetic average is the most commonly used, in spite of the fact that it provides higher values. Nevertheless, apart from its theoretical suitability, the average to be used will be conditioned by the values of the variables considered and by the rescaling or standardisation carried out, given that in order to use the geometric average correctly, only positive values can be used.

PRESENTATION OF THE RESULTS

Following what was said before, the procedure used to make a synthetic gender indicator starts with the obtaining of the individual indices, G1 and G2, for each of the variables that represent the areas of interest considered in this work. Subsequently we proceed to normalise the above mentioned partial indicators and later aggregate them by area. As a result, each will have a synthetic gender index. The same procedure is applied to obtain the general synthetic indicator, with the difference that the values to be added up are the five synthetic indicators calculated for the five areas taken into account.

Among all the alternatives handled we will comment on those that in the current circumstances have clearly proved to be better at reflecting the characteristics of the phenomenon analysed. Thus, the modelling carried out can be summarised by the scheme shown in Figure 1.



Figure 1: Description of the model

We will begin by discussing that which assigns the same weight to all partial indices. In this case, the composite indicator, both those referring to each area and also the general indicator, is obtained as a simple arithmetic average of the partial indices. As summary we show the graphs below (Figures 2-5), that represent the synthetic indices obtained as detailed previously, where not only is it possible to extract information about the general trend of every aggregate, but also about the dimensions that have the greatest influence on the evolution the overall index (G.I.).



Figure 2: G1 normalised - unitary weights



Figure 3: G2 normalised - unitary weights



Figure 4: G1 standardised - unitary weights



Figure 5: G2 standardised - unitary weights

Another alternative used to obtain the composite indicators has been to assign weights derived by Principal Component Analysis (PCA) to the various data series this indicator comprises. This method allows us to detect existing correlations between the normalised partial indices gathered in one dimension and the proper dimension in itself. These correlations are summed up in factors that provide a common variance and facilitate the weight of the involvement that each partial index has in the aggregate.

A very simple change of scale of the coefficients of the component matrix, making its sum equal to one, provides the weights used to calculate the aggregated indicators, obtained in this case as a weighted arithmetic average of the partial indicators. The synthetic indices for each dimension will be added up in the same way, giving each of them a weight provided again by PCA, obtaining thus the overall index. Here we introduce (Table 1) the different weights obtained for G1 and G2, as well as for each of the normalisation methods applied (minimal rescaling, N, and standardisation, S):

Table 1: Weightings obtained through PCA

	G1-N	G2-N	G1-S	G2-S
Power	0,27	0,27	0,19	0,20
Social assistance	0,18	0,13	0,16	0,14
Education	0,16	0,26	0,20	0,21
Activity	0,11	0,06	0,23	0,23
Healthcare	0,28	0,28	0,21	0,22

As we can see, there are significant differences here, mainly concerning the type of normalisation undertaken; hence the results obtained have been quite different, as Figures 6-9 show.



Figure 6: G1 normalised-PCA weights



Figure 7: G2 normalised-PCA weights



Figure 8: G1 standardised - PCA weights



Figure 9: G2 standardised - PCA weights

From the figures included in this epigraph we can immediately and easily interpret the results obtained. In summary, we end up by saying that according to the choice of indices G1 and G2, results do not register significant differences. Nevertheless, the different procedures of normalisation and assignment of weights applied will lead us to very disparate results, both in the contribution of each dimension to the synthetic indices and also in the proper trend of these indicators. As regards minimal rescaling, significant differences are not observed between the weighting systems used, whereas in case of the standardisation these differences are quite marked. In this sense, we could say that the method based on minimal rescaling is more robust when dealing with outliers than the method based on standardisation, and it is also less dependent on the weightings of each indicator.

CONCLUSIONS AND FURTHER RESEARCHS

Gender indicators are important, not only to promote policies focused on overcoming the lack of parity and to review their impact, but also because gender equality plays a vital role in socioeconomic development.

In the model proposed to obtain these indicators, various dimensions measured on different scales must be combined, which means choosing from the various methods available to normalise, weight and aggregate data. Therefore, in light of the uncertainty associated to the model and the decisions taken, which are to a certain extent subjective, we believe it is worth carrying out a sensitivity and uncertainty analysis to capture extant plurality.

After identifying the main factors that affect the variability of the synthetic index, it is necessary to further the research that takes us to the quantification and classification of the above mentioned sources of change. A combined analysis of simulation, uncertainty and sensitivity, would allow us to propose a certain number of groups of acceptable alternative weightings along with a measurement of their permissible variation. All of this would contribute positively to the necessary consensus among professionals in this issue, in order to carry out homogeneous research that facilitates comparability.

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FINANCIAL ANALYSTS IMPACT ON STOCK VOLATILITY. A STUDY ON THE PHARMACEUTICAL SECTOR

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KEYWORDS

Financial analysts, news arrival, pharmaceutical companies, Markov Regime Switching model.

ABSTRACT

Financial analysts play a key role in distinguishing which news are relevant for the valuation of a particular asset, and the changes in their recommendations are signals of new information in the market.

This paper studies the impact those *buy* or *sell* recommendations have on volatility instead of the traditional focus on prices. Twenty stocks from pharmaceutical sector in NYSE are daily tracked for five years along with the recommendations given by financial analysts.

We have modeled stock returns by a Markov Regime Switching model as in (Schaller and van Norden, 1997) and found two states of low and high volatilities. We have also found strong evidence that the probability of being in the estate of high volatility increases when a Financial Analyst changes his recommendation.

INTRODUCTION

The aim of this paper is analyzing the impact on financial markets of the public recommendations given by Financial Analysts (FA). In this sense, the return and volatility of stocks are modeled by a Markov Regime Switching (MRS) Model, founding that transition probabilities between volatility regimes are dependent to changes in the recommendations of FA.

In a efficient market, share prices reflect the correct valuation with the available information. As a corollary, quote changes would be a consequence of the market reaction to the appearance of some relevant news. Unluckily, the identification of relevant news to the evaluation of the market is not straightforward. Although (Fama et al., 1969) concluded that the information is quickly incorporated in the prices and it is not possible distinguish between the non expected part of the news from the expected one, several papers try to find the incidence of the arrival Ricardo Gimeno Bank of Spain Alcala, 48 28014 Madrid, Spain Email: ricardo.gimeno@bde.es

of news in returns. For example, (Pearce and Roley, 1985) analyzes the reaction of quotations to the announcements about monetary supply, inflation, economic activity and the discount rate. Through the expected part of the announcements is possible to test the Efficient Market Hypothesis (EMH) because only the surprise part of the announcement moves prices and in addition, the non-expected part related to monetary policy have a significant effect. So, the difficult point is to distinguish the anticipated part of any news (Pearce and Roley, 1985).

Precisely, the role of FA is collecting all relevant information about an asset as well as evaluating its impact on the price, sending recommendations to the agents. So, changes in FA assessments can be seen as a proxy of the entrance of new and relevant information to the market. They also act as amplifiers of any announcement, spreading their knowledge among actual and potential investors, and therefore affecting the behavior of the asset price.

As stated by (Womack, 1996), the revision of the FA recommendation means that they have analyzed public available information and have reached the conclusion that the present price of the share is not correct. This author also finds a strong evidence that stock prices are significantly influenced by these changes in financial recommendations.

In fact, the companies englobed in the pharmacentrical and biotechnological sector in the USA are highly sensible to news and announcements such as the impact of the decisions about commercialization of a new medicine made by the Food and Drug Administration (FDA) because it could have serious effect on future cash flows. This feature makes them specially suited for the purpose of the present paper, where technical knowledge is needed for distinguishing the possibilities of new drug developments and their value for the company. Pharmaceutical sector has been studied through many points of view, most of them referred to aspects such as regulation (Danzon and Chao, 2000; Philipson, 2002), about the financial valuation of patents (Grabowski and Vernon, 2002) or drug development costs, such as (Grabowski and Vernon, 1990; Berndt, 2002; DiMasi et al., 2003). However, we cannot find so much lit-

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) erature that studies the pharmaceutical sector and its stock exchange characteristics. This paper contributes to the analysis of this particular industry in this aspect.

Nevertheless, measuring the impact of FA recommendations previously requires to impose some hypothesis about the stochastic model governing the behavior of both financial asset's returns and volatilities. In this sense, a mixture of two or more normal distributions is often enough to account for typical skewness and leptokurtosis on returns (Kon, 1984). If the arrival of new information to the market makes greater volatility than in the absence of news, then this behavior would be reflected in two different distributions, one with low variance for the moments of no news and another one with higher variance when announcements are made and markets react to new information.

Additionally, we have to take into account a number of stylized facts about volatility of financial asset prices such as volatility clustering, mean reverting and persistence that has led to models such as the family of ARCH models (Engle, 1982; Bollerslev, 1986) or Markov-switching models introduced by (Hamilton, 1989, 1990). The regime-switching modeling approach was initially proposed as a characterization for economic and financial time series, in order to identify two separated regimes in business cycles. An extension of Hamilton's approach have been used to describe and analyze stock market returns in order to identify two regimes either in mean, variance or both. Some important papers that have used these technics to examine stock market returns are those of (Turner et al., 1989; Hamilton and Susmel, 1994; Schaller and van Norden, 1997).

In the case of (Turner et al., 1989), using S&P monthly index data for the period 1946 - 1989, they consider a Markov switching model in which either the mean, the variance or both may differ between two regimes with univariate specifications with constant transition probabilities. (Hamilton and Susmel, 1994) propose a model with sudden discrete changes in the process that governs volatility. They find that a Markov switching model provides a better statistical fit to the data than ARCH models without switching. (Schaller and van Norden, 1997), in a result close to (Turner et al., 1989), extend their approach in several aspects, i.e. examining whether stock market returns are predictable, even after accounting for Markov switching behavior, as well as whether the transition probabilities of the Markov chain vary over time in response to changes in economic variables. In particular, they look at whether the transition probabilities are influenced by the price/dividend ratio finding an asymmetric response to the past price/dividend ratio.

This paper has modeled stock returns by a Markov Regime Switching model as in (Schaller and van Norden, 1997) to twenty companies during five years along with the recommendations given by FA. We have found two states of low and high volatilities and strong evidence that the probability of being in the estate of high volatility increases when a FA changes his recommendation. Traditionally, literature has concentrated on the impact of FA recommendations on prices and the novelty is that we concentrate on the analysis of the impact of FA recommendations on volatility.

So, a MRS model would allow us to reproduce the main characteristics of stock returns, along with the identification of periods of low and high volatilities. The probabilities of being in each regime can be linked to the chances of appearance of new information in the market at an specific moment, and thereafter, FA recommendations would modify such probabilities.

The rest of the paper is organized as follows: in section we describe the sector selected and the data collected for our analysis. In section , MRS models are estimated founding evidence of different volatility regimes. FA recommendation are added to the model in section while section concludes.

DATA DESCRIPTION

The Pharmaceutical Sector

The pharmaceutical industry is a dynamic sector because of its capacity to reinvent itself in the face of changing market models and government regulation. Currently, the industry is seeking to improve its results from an increasing demand from an ageing population, at the same time that increases its investments in R&D. In particular, genomic research could generate new therapeutic and diagnose products in the next years. As part of this effort, the leading pharmaceutical companies are aggressively moving to form joint-ventures with small biotechnological companies to develop new generations of drugs.

Although these developments involve important challenges and strong investment in risky projects, the pharmaceutical industry is a healthy and profitable one. A great share of the global pharmaceutical market is controlled by companies that are quoted in the New York Stock Exchange, making it an appropriate market to follow.

We can find in the literature several papers that study the process of the life cycle of the discovery and development of new drugs (Grabowski and Vernon, 2002; Berndt, 2002; DiMasi et al., 1991), or the average cost of developing an innovative new drug (DiMasi et al., 2003). However, we cannot find papers that analyze the evolution of this sort of companies in stock markets.

All of these companies depend on the last decision from the FDA, and the not approval in an intermediate phase involves the huge costs that the company will have to assume. Once the FDA is next to announce its decision, rumors and news appear making stock prices to vary widely. FA base their recommendations on the successes and failures of the company, given that the FDA approval of a new drug will ensure new cash-flows for the company.

Stock Returns and Volatilities

The New York Stock Exchange (NYSE) defines companies to be part of the pharmaceutical industry if they are manufacturers of prescription or overthe-counter drugs, such as aspirin or cold remedies. Since 2004, this sector has its own index called *NYSE Health Care Index*. This index includes companies classified in the Health Care sector according to the Industry Classification Benchmark.

Companies included in this index are pharmaceutical and biotechnological that have an important weight in the market capitalization of this sector. The market capitalization in march 2008 was 1246.3 billion dollars, where the 74.7% has an American origin. The five more important companies included in this Index in 31st July 2006 are Johnson&Johnson (9.82% weight), Pfizer Inc. (7.97%), GlaxoSmithKline PLC (7.15%), Novartis AG (6.91%) and Merck (6.51%).

For the present paper we selected the pharmaceutical and biotechnological companies that quoted in the NYSE in January of 2007, during the period 2001 to 2005. We obtained from NYSE/TAQ the closing quotations data. We have chosen those companies with more than 400,000 operations in order to assure they are liquid enough to be covered by a sufficient number of FA following the companies, and the prices correspond to efficiently-enough markets. The final sample of companies have 20 pharmaceuticals and 3 biotechnologicals companies.

Financial Analyst Recommendations

On the other hand, we obtained recommendations of individual analysts jointly with their corresponding dates and the consensus recommendations. This information were not available in all the detail required for all companies selected and this is the reason why some of the original companies had been droped from the sample. So, the companies finally analyzed have been 18 pharmaceuticals and 2 biotechnological companies. All of these information have been obtained from I/B/E/S. As each house of analysis has a different category in its recommendations, I/B/E/S turn all the data to a single category with 5 different levels, assigning to each one a numerical value: (1)strong buy, (2) buy, (3) hold, (4) under-perform and (5) sell. In general they are biased to positive recommendations founding very few selling recommendations, although this can be sensible to the period considered. For example, in the case of Novartis,



Figure 1: NVS Individual recommendations over prices and returns

there are more recommendations with values 2 (buy) and 3 (hold).

In a first approach, we can see in Figure 1 each individual recommendation over prices, returns, variance and volume for Novartis. Dashed green color with a star represents the case of a recommendation improvement respect to the previous, in solid red if it is worse and in dotted black if it is equal.

We encoded the values of the recommendations to move in the range -2 to 2. This five values corresponds to: strong sell (-2), sell (-1), hold (0), buy (1) and strong buy (2). We have made some new variables in order to test the effect of the recommendations on stock returns. These new variables are the following:

- *Recommendation*: Dummy variable indicating if this day a new analyst recommendation has been published. If this is the case, then it could imply higher volatility in the stock, since this new information will require the market to react.
- Value: Value of the new recommendation. The five possible values correspond to: strong sell (-2), sell (-1), hold (0), buy (1) and strong buy (2). It will take into account if the sense of the recommendation has a differential effect on returns (i.e. reactions are stronger after selling recommendations).

- Absolute_value: Absolute value of the new recommendation. It makes no differences between sell or buy orders, just the intensity of the recommendation (buy/sell, 1 or strong buy/strong sell, 2). This variable tries to capture the sensitivity of strong recommendations.
- Variation: It is the change in the value of the recommendation of the analyst with respect to his previous recommendation value. This variable takes into account that the effect on the market will be different if an analyst changes from buy to sell or viceversa, or if he publishes a new recommendation but maintains it as buy or sell.
- $N_{analysts}$: Number of analysts that follows a company. This variable changes along the sample and proxies the power of a given analyst. If very few analysts track a given company, the recommendation given by one of them has greater impact than would have had if he just was one more of a pretty crowd.
- *Consensus*: Daily mean of the last recommendations made by each analyst. It represents the mean of the analysts feelings about the company. The higher the value of this variable, the higher the recommendations to buy and viceversa.
- *Consensus_change*: Difference of the Consensus with respect to previous day. It takes into account that the importance could be not in the value of the recommendations given, but on the changes produced.
- *Absolute_consensus_change*: Absolute value of Consensus_change. The importance is given in this variable to the intensity of the change in consensus and not to the sense of the movement.
- Agreement: Standard deviation of the recommendations on the Consensus. A value 0 means that all analysts agree in the recommendations, and an increase in this variable indicates a higher degree of disagreement. The lower the value of this variable would imply less uncertainty about the company and lower volatility in the stock.
- Agreement_change: Differences in the value of variable Agreement from previous day. It indicates a momentum of increasing or decreasing uncertainty.
- *Absolute_agreement_change*: The absolute value of previous variable *Agreement_change*. It gives the intensity in the increase or reduction on uncertainty never mind the sense of this movement.

 Table 1: Descriptive statistics

	CV	skew	kurt	JB (pv)
Abbott Laboratories (ABT)	107.6	-0.8	14.4	6918.9(0)
Allergan Inc. (AGN)	155.8	-0.1	6.1	501.4(0)
Alpharma Inc. (ALO)	118.1	-0.2	31.4	42144.4(0)
AstraZeneca Group (AZN)	511.3	-0.5	13.2	5536.4(0)
Bristol Myers Squibb (BMY)	20.5	-1.3	13.2	5865.0(0)
Pharmaceuticals, Inc. (BRL)	41.4	-0.2	5.8	430.7(0)
Biovail Corporation (BVF)	91.7	-0.6	12.2	4537.1 (0)
Applera-Celera (CRA)	36.1	0.4	5.2	278.0(0)
Charles River Lab (CRL)	60.8	-0.5	9.7	2370.5(0)
Genentech, Inc (DNA)	43.3	1.8	28.1	33387.4(0)
FOREST LABS INC (FRX)	115.2	-0.4	7.6	1139.9(0)
GlaxoSmithKline (GSK)	193.5	-0.0	5.4	314.4(0)
Johnson & Johnson. (JNJ)	105.7	-1.4	25.2	26186.1 (0)
King Pharmaceuticals (KG)	47.4	-0.9	15.9	8816.2 (0)
Eli Lilly and Company (LLY)	43.2	0.0	5.1	231.4(0)
Merck & Co Inc. (MRK)	22.8	-3.4	56.3	150400.9(0)
Medicis Pharmaceutical (MRX)	207.6	0.1	6.5	644.1(0)
Mylan Laboratories (MYL)	44.2	-0.5	11.0	3394.2(0)
Novartis (NVS)	109.3	0.3	6.6	713.7 (0)
Pfizer Inc. (PFE)	32.1	-0.4	7.2	963.8 (0)
Pharmaceutical Resources (PRX)	27.6	-1.1	28.4	33827.2(0)
Schering Plough Corp. (SGP)	27.5	-0.8	7.8	1306.1(0)
Watson Pharmaceuticals (WPI)	80.1	-6.2	126.7	805521.7 (0)

These variables have been defined for all the companies in the sample of section . With the data on stock returns and recommendations we can define a model that relates both set of variables.

REFERENCE MODEL

Normality hypothesis is usually rejected in the context of financial asset returns. Since the works of (Mandelbrot, 1963) and (Fama, 1965), three characteristics are highlighted to diverge from a gaussian distribution.

- 1. Extreme values in the distribution. The tails of the distributions concentrate more probability than is supposed on a Gaussian distribution.
- 2. Extreme movements are more frequent in the left side of the distribution, as a consequence of market's higher sensibility to bad news.
- 3. Clusters of volatility. Days with high volatility tends to be followed by high volatility also in next days.

The first feature leads to a leptokurtic distribution, while the second one to the presence of skewness in the distribution. This abnormalities are usually attributed to outliers that are distributed as fat tails.

As can be seen in Table 1, skewness coefficients are mostly negative and kurtosis values are greater than 3 in all cases. Both are evidences of non-gaussian distributions, a fact confirmed by Jarque-Bera test, presenting pvalues close to zero for all the companies, rejecting the null of normality.

Moreover, in financial returns we can observe persistence in volatility and volatility clustering, mean reverting. The study of the autocorrelation function for Novartis shows, weak evidence of dependence on the mean (Figure 2 a.), assuming a constant mean. At the same time, in the correlogram of the squared returns (Figure 2 b.s) all the autocorrelation coefficients are positive and with significant and slow pos-



Figure 2: a. NVS Autocorrelation function for returns



b. NVS Autocorrelation function for squared returns

itive decay which indicates an important dependence of past values of the volatility.

Observations of this type in financial time series have led, in many cases, to the use of ARCH family models in financial forecasting and derivatives pricing, such as ARCH (Engle, 1982) and GARCH (Bollerslev, 1986) models. The main idea behind these widely-used models is that volatility is dependent upon past realizations of the asset process and related volatility process. This is a more precise formulation of the intuition that asset volatility tends to revert to some mean rather than remaining constant or moving in monotonic fashion over time.

Regime Switching Model

Previously to the analysis of recommendation impact on stock returns, we need a benchmark model for the later variable. Financial returns are usually modeled using stochastic volatility models like GARCH family of (Engle, 1982) and (Bollerslev, 1986). Although this models allows to take into account volatility clustering they are not fully able to explain fat tails and skewness. Some modifications on this models could help to introduce such features in the model but had the drawback of their increasing complexity.

Alternative modeling of return distribution via Extreme Values Theory (see (Embrechts et al., 1997) for a detailed description). has similar disadvantages and becomes difficult to conciliate them with financial theory. Nevertheless a simplest way of reaching similar results are the mixture of normal distributions, each one representing a different situation of the market.

We can find the origin of this model in the work of (Clark, 1973), that uses the concept of subordinated

stochastic process and interpreted the leptokurtic behavior as a signal that the negotiation activity is not distributed uniformly during the period of negotiation.

Another important work that applied a mixture of normals to explain the indicated problems (fat tails, kurtosis and asymmetry) is the one of (Kon, 1984). He proposed a mixture of normal discrete distributions and indicated that although the hypothesis of a model with stationary normal distribution is empirically rejected, the gaussian hypothesis has great importance in financial theory.

The model presented by (Kon, 1984) was formed by a discrete mixture of four normal distributions for stock-exchange returns of 30 shares quoting in the Dow Jones. His results showed that it was a superior model than the student alternative, allowing to explain the asymmetry and kurtosis observed in the analyzed data. (Gonzalez and Gimeno, 2006) also showed that with a mixture of just two normal distribution it is possible to explain leptokurtosis and skewness of 30 worldwide stock indexes.

Nevertheless, a mixture of normal distributions is not able to explain the clusters of volatility in stock returns. In this sense, (Schwert, 1989) consider a model with two normal distributions with different variance in which transitions between variances are governed by a two-state Markov process. (Turner et al., 1989) generalized the model to allow both mean and variance to change between regimes, capturing the skewness in the distribution with different impacts on mean returns of states of low or high volatility. Finally, (Hamilton and Susmel, 1994) showed that a Markov regime switching (MRS) model provides a better statistical fitting than ARCH models.

This MRS model, originally proposed by (Hamilton, 1989), would allow us to distinguish the existence of different regimes in financial assets. Although MRS models can be quite flexible in the mean equation of each regime, we have selected a restricted version with a constant similar to (Turner et al., 1989),

$$r_{t} = \begin{cases} \mu_{1} + \epsilon_{1t} & if \\ \mu_{2} + \epsilon_{2t} & \epsilon_{2t} - N(0, \sigma_{2}) \end{cases}$$
(1)

Model 1 has two different regimes $(s_t = 1 \text{ and } s_t = 2)$, one of them with low volatility (σ_1) and other one with high volatility (σ_2) that could be linked to the turmoil after the entrance of new information on the market. Skewness would be consequence of different means $(\mu_1 \text{ and } \mu_2)$ between regimes, since markets tends to react stronger upon bad news.

Each of the regimes in equation 1 are normally distributed, so the model can be considered as a mixture of normal distributions. Additionally, state variable (s_t) is a Markov chain with a transition matrix P (equation 2) that gives the probabilities of being in any regime conditioned to the regime in previous period.

$$P = (p_{ij}) = \begin{pmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{pmatrix} = \begin{pmatrix} p_{11} & 1 - p_{11} \\ 1 - p_{22} & p_{22} \end{pmatrix}$$
(2)

In equation 2, p_{11} denotes the probability of being in regime 1 ($s_t = 1$), conditioned to having been also in regime 1 the day before ($P(s_t = 1|s_{t-1} =$ 1)), whereas p_{22} plays the same role for the second regime. Values of p_{22} , linked to the regime of high volatility, close to one will implied volatility persistence and produce clusters of volatility as the ones found in financial time series.

Parameter estimations of both equations 1 and 2 are obtained via maximum likelihood (see (Hamilton, 1989)). Nevertheless, the function we have to optimize is not linear, being sensible to the initial parameters in the model. To accelerate the optimization process we select initial values for the parameters (μ_1 , μ_2 , σ_1 , σ_2 , p_{11} , p_{22} and the probability of being on regime 1 in the first period p_0), following the methodology of (Gonzalez and Gimeno, 2006).

We roughly identify the days of high volatility to compute both μ_i and σ_i in each regime. The methodology consist in an iterative procedure that successively test normality hypothesis though Jarque-Bera test (Jarque and Bera, 1980) and drop the data with higher absolute daily returns, until a sub-sample is reached where normality hypothesis is not rejected. The returns in this sub-sample are initially considered as generated by the distribution with lower volatility of regime 1, whereas the dropped ones would be identified as days with high volatility.

Through this procedure we will obtain two groups of returns, that can be assigned to regime 1 and 2. Once we have separate the data, we can obtain the initial mean and variance values for each of the states. Transition matrix is also easily estimated once we have tentative regimes for each day, whereas p_0 is set to be equal to 0 or 1 depending on the first return classification.

This values are just tentative, and final parameters are estimated via maximum likelihood (Table 2). As can be seen, regime 2 is assigned to the distribution with higher standard deviation (tipically three times higher). The probability of remaining in the same regime are also high in both states, and reinforce the evidence on clusters of volatility.

Figure 3 represents the stock returns of Novartis plotted with different color depending on the results of the probabilities of being in each regime. It is possible to see how the probabilities of being in the first regime (in green color) or in the second one (in red color with star points) change along the time and coincide with the periods of high and low volatility in the returns.

Table 2: Estimated values of MRS parameters

	μ_1	σ_1	μ_2	σ_2	p_{01}	p_{11}	p_{22}
ABT	0.01%	1.14%	-0.07%	2.77%	1.00	0.97	0.92
ALO	0.05%	2.32%	-0.57%	11.70%	1.00	0.96	0.36
AGN	0.03%	1.02%	0.02%	2.68%	0.00	0.94	0.90
AZN	-0.03%	1.30%	0.15%	3.25%	1.00	0.97	0.89
BMY	-0.01%	1.04%	-0.20%	2.62%	0.00	0.98	0.96
BRL	0.07%	1.40%	0.03%	3.17%	1.00	0.93	0.83
BVF	0.08%	1.94%	-0.47%	5.87%	0.00	0.92	0.67
CRA	-0.10%	2.29%	-0.12%	4.21%	0.00	0.99	0.98
DNA	0.06%	1.76%	0.22%	4.94%	1.00	0.97	0.92
FRX	0.06%	1.51%	-0.10%	3.71%	0.00	0.92	0.71
GSK	-0.01%	1.12%	0.00%	2.36%	1.00	0.98	0.95
JNJ	0.01%	0.87%	0.04%	2.21%	0.00	0.96	0.89
KG	0.10%	1.67%	-0.49%	5.20%	0.00	0.91	0.74
LLY	-0.05%	1.20%	0.04%	2.47%	0.00	0.98	0.95
MRK	0.02%	1.24%	-0.73%	4.44%	0.00	0.96	0.68
MYL	0.01%	1.34%	0.21%	3.56%	0.00	0.90	0.67
NVS	0.01%	0.99%	0.07%	2.24%	1.00	0.97	0.88
PFE	-0.06%	1.21%	-0.01%	2.82%	0.00	0.98	0.93
SGP	-0.01%	1.42%	-0.20%	3.01%	0.00	0.97	0.94
WPI	0.01%	1.52%	-0.80%	7.72%	0.00	0.96	0.46



Figure 3: NVS Posteriori probabilities over returns

In Table 3 and 4 we present the results of likelihood ratio tests (see (Engle, 1984) for a general description and (Hansen, 1992) for its application on MRS models) on the estimated model for each company. The test on the null hypothesis of equal means in both regimes (column 2) are accepted in all but two companies, as well as being equal to zero (Table 3 columns 4, 5 and Table 4 column 2) in all but one case. This results imply that there is no forecasting opportunity on stock returns, as is generally found in the financial literature. Nevertheless, in the case of σ_i parameters, the null hypothesis is rejected (Table 3 column 3), reinforcing the idea of the two regimes related with low and high volatility. Finally, the null of no regime switching is also rejected in all cases (Table 4 column 3).

In addition, we have proceed to calculate the standardized residuals of the model. When we compare the moments of the original return distribution with the ones obtained from the residuals of the MRS model (Table 5), both skewness and leptokurtosis are dramatically reduced (80%-90% of reduction). In terms of normality, the reduction is even higher in the Jarque-Bera statistic, and in half of the cases the reduction is enough to accept the normality hypothesis.

In Figures 4 a) and 4 b) we present the correlation and partial correlation function for both the residuals of the MRS model as well as the squared

Table 3: LR tests on MRS models (a)

	$\mu_1 = \mu_1$	¹ 2	$\sigma_1 =$	σ_2	$\mu_1 = 0$	$\mu_2 =$	0
ABT	0.21		287.4	***	0.04	0.19	
AGN	0.00		295.4	***	0.41	0.02	
ALO	0.16		345.2	***	0.52	0.14	
AZN	0.61		263.0	***	0.40	0.47	
BMY	2.06		228.7	***	0.06	2.63	
BRL	0.04		157.1	***	1.26	0.01	
BVF	1.63		200.0	***	1.12	1.33	
CRA	0.00		156.7	***	1.32	0.34	
DNA	0.31		418.5	***	0.75	0.61	
FRX	0.34		160.1	***	1.16	0.15	
GSK	0.00		204.6	***	0.02	0.00	
JNJ	0.04		303.7	***	0.16	0.10	
KG	3.17	*	240.5	***	2.26	2.46	
LLY	0.31		181.8	***	1.43	0.06	
MRK	3.64	*	265.0	***	0.18	3.60	*
MYL	0.18		131.4	***	0.01	0.34	
NVS	0.12		124.2	***	0.08	0.21	
PFE	0.06		258.3	***	1.89	0.00	
SGP	1.32		199.9	***	0.00	1.72	
WPI	0.82		241.7	***	0.07	0.81	

With ** for those values with pvalue< 0.01, with ** for pvalue< 0.05 and * for pvalue< 0.1

Table 4: LR tests on MRS models (b)

	$\mu_1 = \mu_2 = 0$	$s_t(1) =$	$s_t(2)$
ABT	0.22	287.5	***
AGN	0.48	303.6	***
ALO	0.62	587.7	***
AZN	0.78	263.0	***
BMY	2.76	369.7	***
BRL	1.52	157.3	***
BVF	2.00	357.5	***
CRA	1.80	157.8	***
DNA	1.50	419.7	***
FRX	1.16	197.7	***
GSK	0.02	204.6	***
JNJ	0.33	303.9	***
KG	4.01	417.8	***
LLY	1.43	183.3	***
MRK	3.64	497.7	***
MYL	0.95	245.0	***
NVS	0.37	190.6	***
PFE	1.94	258.6	***
SGP	1.80	201.0	***
WPI	0.84	707.3	***

pvalue< 0.01, with ** for pvalue< 0.05 and * for pvalue< 0.1

Table 5: Normality test

	SKEWNESS		KURT	OSIS	JARQUE-BERA TEST			Г
	r1	rs	r1	rs	r1		rs	
ABT	-0.8	-0.2	14.4	4.1	6918.9	***	68.4	***
AGN	-0.1	0.0	6.1	2.7	501.4	***	4.8	*
ALO	-0.1	0.0	31.5	2.7	42144.4	***	3.4	
AZN	-0.5	-0.2	13.3	3.4	5536.4	***	12.5	***
BMY	-1.3	-0.4	13.3	4.9	5865.1	***	214.5	***
BRL	-0.2	0.0	5.9	2.6	430.7	***	6.8	**
BVF	-0.6	0.1	12.3	2.8	4537.2	***	4.3	
CRA	0.4	0.2	5.2	3.2	278.0	***	10.7	***
DNA	1.8	0.4	28.1	5.7	33387.5	***	418.9	***
FRX	-0.4	-0.0	7.6	2.6	1139.9	***	9.3	***
GSK	-0.0	-0.0	5.5	2.8	314.5	***	2.2	
JNJ	-1.4	-0.4	25.3	6.1	26186.1	***	524.7	***
KG	-0.9	-0.1	15.9	3.4	8816.2	***	11.2	***
LLY	0.0	-0.1	5.1	2.6	231.4	***	11.4	***
MRK	-3.4	-0.1	56.3	4.2	150400.9	***	82.9	***
MYL	-0.5	-0.2	11.0	3.1	3394.2	***	7.9	**
NVS	0.3	0.1	6.7	2.7	713.7	***	4.1	
PFE	-0.4	-0.1	7.3	2.9	963.8	***	1.9	
SGP	-0.9	-0.2	7.8	3.4	1306.1	***	15.1	***
WPI	-6.2	-0.1	126.7	3.8	805521.8	***	39.2	***

With * * * for those values with pvalue < 0.01, with ** for pvalue < 0.05 and * for pvalue < 0.1 r_1 represents stock returns while r_s are MRS standardized resids



Figure 4: a. NVS Autocorrelation function for standardized RMS resids



b. NVS Autocorrelation function for squared standardized RMS resids

residuals. When compared with the ones obtained from the raw returns (Figures 2 a) and 2 b)) it is possible to see that although correlogram on the original variables are quite similar, in the case of the squared variables, that in the case of returns indicates the presence of conditional heterokedasticity, this evidence disappear in the residuals of the MRS model, indicating that GARCH modelling is no longer needed. Similar results are obtained for the other companies.

THE EFFECT OF FA RECOMMENDA-TIONS

Once we have a valid model to represent stock returns, we can measure the impact on volatility of FA recommendations. We follow (Schaller and van Norden, 1997), and consider that the transition probabilities on equation 2, instead of being constant, can be set to be a function of some exogenous variables,

$$p_{11} = P(S_t = 1/s_{t-1} = 1, A_t) = \Phi(A_t\beta_1)$$

$$p_{22} = P(S_t = 2/s_{t-1} = 2, A_t) = \Phi(A_t\beta_2)$$
(3)

where A_t is, in our case, a vector containing the recommendation variables defined in section ((Schaller and van Norden, 1997) used the past price/dividend ratio) and $\Phi(\cdot)$ is a function that returns the cumulative probability of a normal distribution. Then the probabilities on (3), becomes Probit models (In fact, we used Probit estimations as initial values of the final model), and the transition matrix is redefined,

$$P = \begin{pmatrix} \Phi(A_t\beta_1) & 1 - \Phi(A_t\beta_1) \\ 1 - \Phi(A_t\beta_2) & \Phi(A_t\beta_2) \end{pmatrix}$$
(4)

Since A_t vector contains eleven variables, β vectors would add 22 extra parameters to the estimation.

	FA rec				
ABT	64.321	***			
AGN	89.747	***			
ALO	63.090	***			
AZN	44.512	***			
BMY	84.160	***			
BRL	79.139	***			
BVF	117.595	***			
CRA	57.173	***			
DNA	73.213	***			
FRX	81.531	***			
GSK	42.240	***			
JNJ	62.860	***			
KG	82.656	***			
LLY	53.203	***			
MRK	39.542	**			
MYL	70.134	***			
NVS	48.862	***			
PFE	43.515	***			
SGP	56.298	***			
WPI	64.971	***			
Where					

Table 6: LR tests on the influence of FA over transition probabilities

> * * * indicates pvalue< 0.01, ** for pvalue< 0.05

and * for pvalue < 0.1

In Table 6, we present the LR test under the null of no effect of FA recommendations in the volatility regime. As can be seen, in all of the cases the null is rejected, and strong evidence is found of the effect of FA on the volatility. This result suggest that either the FA has direct effect on the market or that he has reach in its recommendation the same conclusion the market does.

CONCLUSIONS

In the present paper we have analyzed the effect of FA recommendations on the market volatility of Pharmaceutical and Biotechnological companies. This paper contributes to the literature because analyzes the sector and its stock exchange characteristics. Moreover, we study the impact of FA recommendations on volatility instead of the traditional literature that focuses on prices.

We have found in all of the 20 companies analyzed strong evidence of correlation between FA recommendations and changes in volatilities. This result may point out to the role of FA to extend new information about a company to the market, since such event is usually linked to higher volatility in a price discovery process.

We have also found that a mixture of simple two normal distributions with the same mean but different variance, with probabilities governed by a Markov chain (MRS model), is able to capture the main features of financial assets in a meaningful model. A MRS model is considerably more parsimonious than alternatives like GARCH models and extreme values distributions, but at the same time is able to take into account volatility clustering, leptokurtosis and skewness in financial returns.

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MODELLING THE VARIABLES THAT INFLUENCE THE SCHOOL PERFORMANCE IN THE MADRID MUNICIPALITIES

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ABSTRACT

The evaluation of the school performance is a very important strategic field due to the great amount of public and private resources invested by the society in education. State and regional governments undergo several tests and surveys which try to measure the levels of learning attained by their students. While there is a rich literature on the main inputs that explain the school performance at the State level, the concrete determinants at the municipality level –as immigration and the local budget in education– have not been widely addressed.

This paper estimates a cross-section data model using the results of the specific test developed by the Madrid Regional Government in the academic course 2007-08. Our cross-sectional dataset includes 617 schools in 130 municipalities in the surrounding area of Madrid, using data at municipal and school levels. From our study we detect two variables that have an important impact in the scholastic results, the specific characteristics of each school, where the number of foreign students, the ownership of the school, and the municipality expenditure effort in education stand up. The analysis shows the capacity of regional and local government to overcome the education outcomes.

INTRODUCTION

The economic analysis of education has studied the microeconomic effects of education in the labor markets and the workers income, and the macroeconomic influence of education in the economic growth of nations. Nevertheless there is a specific literature that focuses on the analysis of the educational system itself, and the efficiency of schools to educate and bring up students. This literature looks education and schools as a production function, where the inputs, as the students' personal characteristics and their socio-economic and school environment, produce an output of education achievement. The production function approach to education establishes two main groups of inputs, the personal and environment characteristics of the students (intelligence, family income and culture), and the characteristics of the school and the teachers. Within this second group of characteristics, the government tries to improve the students' achievement by giving more resources to schools.

In 1966, the U.S. government promoted a study about the educational resources in the country, known as the "Coleman Report" (Coleman et al. 1966). This study, besides describing the school resources in the U.S., used the education production function to measure the influence of different inputs in the students' achievement. The conclusion of this study was that differences in school resources have little influence in students' outcome, whilst family background and peers' characteristics are more important. The "Coleman report" was the beginning of a literature that uses the production function technique to analyze and measure the factors that influence the students' achievement. This article also opened a controversial debate, not solved up to now, about the influence of the school resources in their students' achievement. Almost all empirical analyses find that the students' personal characteristics and their family and social environment have a decisive influence in their outcome. The controversy focuses on the variables related to the school characteristics. Some authors support the idea of a weak relationship between school resources and students' achievement (Coleman et al. 1966; Hanushek 1986, 1997, 2003). As a reaction of this attitude, other researchers emphasize the relevance of some school resources (Summers and Wolfe 1977; Card and Krueger 1992; Hedges, Laine and Greenwald 1994; Vergestegen

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) and King 1998; Figlio 1999; Dewey 2000; Krueger 1999, 2003). This controversy shows the problems of the education production function analysis related to the available data, its relevance, and the statistical models used to measure its influence.

The literature measures the school outcome using the standardized achievement test scores. Obviously, these tests are not specifically designed to measure the future students' performance in the labor market, and they focus only on basic achievement (usually language and mathematic skills). There is a problematic connection between the present school achievement and the future post-school outcome of these students in the labor market. That is the reason why these tests are more appropriated to some students or jobs than others, and, for example, they tend to be more suitable in the earlier grades. Another problem with these tests is that the individual test score information for each student is seldom available, but only the aggregate information for schools uses to be accessible.

Inputs have also availability problems, so to avoid the temptation of choosing only the available inputs, it is important to classify them and take into account their most important characteristics. The main inputs can be classified in two groups, 1) the socio-demographic characteristics of students' families and peers (income, parental education), and 2) the school organization (class size, administrative expenditure) and teachers characteristics (culture, wages, tenure, experience). There is a third input related to the personal characteristics of the students that define their learning potential. Obviously, a smarter or hard-working student will have a better achievement, thought it is very difficult to measure those capacities. Moreover, all the inputs interact between them and with these innate personal abilities to produce a specific outcome. Besides, the education process is cumulative, so past inputs have some influence in present output. Though it is very difficult to measure all these variables, there is an indirect way to take them into account, by using past outputs (that is, test scores in previous years) as an input of potential output level (Bacdayan 1997; Goldhaber and Dominic 1997).

The input analysis has been concentrated in the school characteristics, trying to measure which of these features are relevant for the output, taking always into account the personal, familiar and peer characteristics. There are a lot of studies about this issues applied to different educational systems, with the problem that their empirical results are very different and problematic to compare because each study uses different variables. Some articles have made compilations of articles that compare the empirical results of different studies, again with varying results. Others have made international comparisons, either using world-wide scholastic performance tests (PISA, TIMSS), or making compilations of different articles from different countries. Once more, the results of these comparisons are varied: while some authors support the fact that influence of school characteristics in students achievement is higher in developing countries than in the developed ones (Fuller and Clark 1994; Glewwe 2002), other researchers maintain the relative irrelevance of school resources in their performance (Hanushek and Luque 2003).

The inconclusive results of the input-output analysis in the educational system show the ignorance of the shape of the education production function. Besides the problems with data availability, the schools are complex organizations that deal with complex agents (students, teachers, parents), so relationships between inputs and outputs are not easy to analyze. Just having more computers or more teachers per student does not assure that the achievement of the students will increase.

In the economic educational analysis, the main efforts to identify the contexts, processes and methodologies that transform educational inputs in students' outcomes, have been made through an increasing sophisticated statistical analysis. If individual data of each student are available, then the researcher can use the Data Envelopment Analysis (DEA), a non-parametric analysis based on models of mathematical optimization (Worthington 2001). This technique overcome the problem of the ignorance of the production function shape (it is not necessary to specify it in the model), and is very appropriate to measure the efficiency of schools resources. But when data are aggregated and it is important to measure the influence of inputs in the school achievement, the econometric or parametric analysis is the best option. However, this second option has also limitations. One is the diminishing returns of inputs when their use is very intensive (non-significant coefficients would reflect then this congestion point but not the irrelevance of the variable). Other problem is related to data aggregation, because aggregate-level correlations have not to be the same as individual-level correlations. For example, some inputs could be more positive for advanced students and others more appropriate for backward ones (Eide and Showalter 1998). One way to overcome this problem is the use of multilevel models, because students are not simple random samples from the population of students, their performance within the same class will be correlated, as will be the performance within the same school or the same district. It must be established the level at which it is measured each of the variables.

In conclusion, the influence of specific inputs on students depends mainly on the characteristics of each educational system. Therefore, next section will analyze the Spanish educational system.
THE SPANISH EDUCATIONAL SYSTEM

The arrival of Democracy in Spain increased the public social expenditures in health, pensions, and education. There is a great interest of governments and society in evaluating the efficiency of these expenditures. Almost all studies find a negative outcome of the Spanish educational system, because the international comparisons studies (the most relevant for the Spanish case is PISA) show bad outcomes of our students in spite of the increasing resources expended in the schools (Fuentes 2009). The main problems are the comparative lower level of the Spanish students, and the higher rates of academic failure and abandon before finishing the secondary school.

The Spanish educational system has some relevant characteristics. One of them is the existence of three types of schools: public schools, controlled by the government and where students do not have to pay tuition, private schools, which have to follow only some simple and general education governmental rules, and a third group of schools, named "concertados", which are private schools that receive government vouchers for most of the student's tuition and imposes a commitment on the part of the school to adhere to certain rules and standards outlined by the government (students-class ratio, students-teachers ratio, academic background of teachers, syllabus, and students draft system). Another outstanding characteristic of the Spanish educational system is that, in the last years, the responsibilities in education have been transferred from the central state to the regional governments.

The decentralization of the Spanish educational system and the previous elimination of the homogeneous academic achievement tests for scholar students, explain the scarcity of individual students' achievement information in Spain. Researchers have used mainly the University Entrance Examination, the only standardized test for all the Spanish students made at the end of the secondary school (San Segundo 1991; Pedraja and Salinas 1996; Mancebón 1998; Mancebón and Bandrés 1999; Muñiz 2000; Seijas 2005; Dios-Palomares et al. 2006), the PISA data on Spanish students (Santín 2006; Calero and Escardíbul 2007), and other indicators when available, like specific tests made in schools by the regional governments (Cordero et al. 2005). All these studies use the DEA analysis to measure the efficiency of the schools. In most of the cases, the sample is a limited number of schools in one specific city or region. All these studies find a close relationship between the student's socioeconomic level and their performance.

Other studies use grouped data and parametric models to investigate some specific characteristics of the Spanish educational system, like the comparison between public and private schools (Calero and Escardíbul 2003; Sancho 2008) and the role of immigrants in the educational system (Salinas and Santín 2007). Both factors are related, given that the concentration of immigrant students in public schools can reduce their achievement.

The Regional Government of Madrid has developed a special test to evaluate the knowledge and capabilities in Mathematics and Language of students in their last year of primary school (12 years old). This test started in 2005 and is made in all the schools of the region. The publication of the results of these tests, grouped by schools, started a controversy because some political parties and labor unions did not like the comparisons between public and private schools that could be derived from the published results. In the next two years the results of the test were not published, and in 2008 were published again. The only study about this test, the one published in 2005, found an important influence of the economic characteristics of the student's district or neighborhood, and the immigration through their massive presence in the public schools in some districts, although it only studied the results of the schools in Madrid city, but not in the rest of the region (Crespo et al. 2006).

Our study uses the academic results of this test in 2008, with 729 schools of the Madrid municipalities, without including schools from Madrid City. The objective is to analyze the main factors that explain the school performance at the municipality level, through not only traditional variables as the socioeconomic context of the student and the school resources, but other variables related to the importance of the municipality where the student live, and some other factors that are in the special context of the regional educational system such as the ownership of the school and the number of immigrants at the school.

METHODOLOGY

By developing a cross-section data model, this paper tries to explain –on a school-by-school basis– the potential variables which can explain the variability of the exam results of the sixth grade of primary education. Cross-section models can be used to analyze the data of a broad sample of individuals, families, enterprises, countries –or, in this specific case, the primary schools in Madrid– in a given year. Therefore, we do not have a temporal dimension.

While the time series analysis must adopt a broad set of econometric tools which are also used in the crosssection analysis, the first one is more complicated because of the usual existence of trends, correlations (and autocorrelations), dynamics, or stationarity, in economic time series.

On the other hand, although some econometric models derive from formal economic models and theories, other

studies are based on non-formal economic reasoning and the intuition. It is the case of the present paper.

Some of the most frequent problems that are observed in the cross-section data analysis are heteroskedasticity, multicolinearity, endogeneity or estochastic regressors. As can be proved, the model developed in this paper, and the results derived from it, are robust enough to the previous problems.

THE MODEL

The present study is based on the 2008 test of the sixth grade of primary education in the schools of the Madrid region. The developed model tries to explain the variability of the results of the examination of the sixth grade of primary education as a result of a set of variables. These variables can be classified in two broad groups:

1) Particular characteristics of each of the schools: available educational resources, students composition (immigrants versus domestic students), and ownership of the educational centers. Under this group we include the following variables per school:

- The student-teacher ratio (stud/teacher)
- The student-computer ratio (stud/computer)
- The foreign students (immigrants)/total students ratio (foreign/total)
- A dummy-variable (0,1,2) which reflects the titularity of the educational centers (titul): public schools, *private schools that receive public funds* (*"concertados" schools), and* private schools, respectively.

2) Economic, geographical and political characteristics of the municipality where the schools are placed: per capita income (Yp), public spending on education over the total public spending of the municipality (edspending), municipality's distance to Madrid City (dist), and two dummy variables which represent the political party in power: PP (that adopts the value of 1 under a Popular Party government and 0 otherwise) and PSOE (which adopts the value of 1 under a Socialist Party government and 0 otherwise).

The econometric specification of the model is the following:

$$\log(grade)_{i} = c + \beta_{1}(stud \mid teacher)_{i} + (1)$$

+ $\beta_{2}(foreign \mid total)_{i} + \beta_{3}(stud \mid computer)_{i} + \beta_{4}(titul)_{i} + \beta_{5}\log(Yp)_{i} + \beta_{6}(edspending)_{i} + \beta_{7}(dist)_{i} + \beta_{8}(PP)_{i} + \beta_{9}(PSOE)_{i} + \varepsilon_{i}$

The empirical analysis is based on the "Knowledge and Capabilities of Mathematics and Language" test developed by the Madrid Autonomous Community in the last four years. We have used the last test made in the course 2007/2008 to 1,270 schools, 541 within the City of Madrid, and 729 in the rest of the municipalities of Madrid Region. The first objective is to compare the municipalities' differences, so we have to erase the schools of Madrid City because it introduces distortions in the analysis. The option of dividing the Madrid's schools into districts is not possible because there are no so many data at this level as at the municipality level. Given the lack of some relevant data at municipal level, the final analyzed sample includes 617 schools.

The data set at the municipality level comes from the National Statistics Institute (INE) and the Municipal Database of the Statistics Institute of the Community of Madrid (ALMUDENA): population age, foreign population, uneducated population, distance to Madrid City, political party governing the municipality, and per capita income level. Education expenditure of each municipality (data from the Minister of Finance) is also included.

The competence in education expenditure is at the regional level (the government of the Community of Madrid), even though each municipality can add expenditures to expand the education effort in its municipality. We have used education expenditure as a percentage of the total municipal budget.

Besides the municipality level data, we have introduced other data at a school level: number of students and foreign students, number of teachers, classes, and computers. All these data are provided by the Education Services of the Autonomous Community of Madrid.

Table 1 shows the *a priori* expected signs for each of the previous variables. On the other hand, Table 2 reports the results of the estimation of equation (1) using WLS.

Students/teacher ratio (<i>stud teacher</i>)	(-)
Foreign students/total students (foreign / total)	(+) or (-)
Students/computer ratio (stud / computer)	(-)
Titularity (titul)	(+) or (•)
Per capita income (<i>Yp</i>)	(+)
Education spending/total spending (edspending)	(+)
Distance from the capital (dist)	(-)
Popular Party government (PP)	(+) or (-)
Socialist Party government (PSOE)	(+) or (-)

Table 1. Expected signs for the model regressors.

Dependent Variable: log(grade) Method: Weighted Least Squares Sample: 1 617 Included observations: 617 Weighting series: 1/log(Yp)

Variable	Coefficient	t-Statistic	Prob.	
С	2.888500	28.07290	0.000)
stud/teacher	-0.001937	-2.266731	0.0238	3
foreign/total	-0.264828	-5.108807	0.0000)
stud/computer	-0.022902	-2.049431	0.0408	3
titul	0.107198	3.740950	0.0002	2
log(Yp)	0.121600	3.587913	0.0004	ŧ
edspending	0.424691	1.924220	0.0548	3
dist	-0.002171	-3.795475	0.0002	2
PP	0.017882	0.787789	0.4311	
PSOE	-0.008827	-0.377415	0.7060)
	Weighted	Statistics		
R-squared	0.642858	Mean depende	ent var	3.072436
Adjusted R-squared	0.637554	S.D. depender	nt var	0.270132
S.E. of regression	0.162629	Akaike info crit	erion	-0.778587
Sum squared resid	16.02766	Schwarz criter	ion	-0.706781
Log likelihood	249.8047	F-statistic		16.01080
Durbin-Watson stat	1.961593	Prob(F-statistic	c)	0.000000

Table 2. Regression results.

All variables, except the dummy variables for the political party governing the municipality (*PP* and *PSOE*), show the expected sign and are significant at the 5% level. It is very relevant to underline the very high significance of variables like the *foreign students/total students* ratio, the ownership of the school (public-private), the per capita income level of the municipality, and the municipality's distance to Madrid City. Finally, the weighted fit of the model is relatively good (R^2 =0.64)

A simple reading of Table 2 shows that:

- The higher the *student-teacher ratio*,
- The higher the *student-computer ratio*,
- The higher the *foreign students/total students ratio*,
- The lower the *per capita income level* of the municipality,
- The lower the *education public spending/total municipal budget ratio*,
- The greater the *municipality's distance* to the capital...
- ...the lower is the average mark for the exam.

On the other hand, it is relevant to emphasize on the existence of a positive and significant relationship between private/"concertados" schools and the average mark of the examination.

Therefore the estimated model is as follows:

 $log(grade)_{i} = 2,8885 - 0.0019(stud | teacher)_{i} + -0.2648(foreign | total)_{i} - 0.0229(stud | computer)_{i} + +0.1071(titul)_{i} + 0.1216log(Yp)_{i} + 0.4246(edspending)_{i} + -0.0021(dist)_{i} + \varepsilon_{i}$

Figures 1 and 2 demonstrate that model residuals do not show any obvious patterns that seem inconsistent with the assumptions of the model.

Sample: 1 617 Included observation	s: 616					
Autocorrelation	Partial Correlation		AC	PAC	Q-Stat	Prob
		1 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 6 17 18 19 20 21 22 23	0.012 0.073 -0.005 0.004 0.028 0.001 0.032 -0.003 0.118 0.012 0.032 0.042 0.042 0.026 0.046 0.026 0.044 -0.010 0.034 -0.045 0.026 0.026	0.012 0.073 -0.007 0.029 -0.000 0.028 -0.003 0.115 0.010 0.042 0.023 0.023 -0.008 -0.004 0.020 -0.052 0.016 0.056 -0.060 -0.037	0.0939 3.4055 3.4226 3.4324 3.9098 3.9100 4.5432 4.5474 13.430 14.090 15.266 17.430 17.400 17.400 17.500 18.245 19.562 19.977 22.254 23.617 23.796	0.759 0.182 0.33 0.488 0.562 0.688 0.716 0.808 0.228 0.228 0.228 0.228 0.229 0.229 0.229 0.229 0.229 0.229 0.229 0.229 0.229 0.229 0.235 0.242 0.242 0.242 0.429 0.449 0.429 0.429 0.429 0.449 0.429 0.449 0.449 0.429 0.449

Figure 1. Model residuals



Figure 2. Model residuals

CONCLUSIONS

This article develops a model that explains the variability of the examination marks of the sixth grade of primary education as a result of two broad set of variables: 1) particular characteristics of each school (available educational resources, students composition, and ownership of the educational centers), and 2) economic, geographical and political characteristics of the municipality where the schools are placed (per capita income level, public spending on education over the total public spending of the municipality, distance to

Madrid City, and the influence of the political party in power).

The cross-section data model is estimated under a Weighted Least Squares (WLS) method for correcting heteroskedasticity, and the model demonstrate that the examination results of the sixth grade of primary education in the schools of Madrid region are negatively related to the available educational resources of each of the primary schools individually considered (student-teacher ratio and student-computer ratio). On the other hand, there is a negative and significant relationship between the proportion of foreign students in the total number of students and the examination grades. The third point to be considered is the existence of a positive and significant relation between private/"concertados" schools and the results of the examination.

Additionally, it must be emphasized the existence of a clear and significant positive relationship between municipalities' economic factors (per capita income level and public spending on education over total public spending) and the results of the exam.

Finally, we can define as a non-expected result the existence of statistically significant relationship between the municipalities' distance to Madrid City and the results reached by the primary school students. Is it maybe the proximity to the capital a factor of major and better access to education and culture for the students of primary schools in the Community of Madrid?

APPENDIX

	ALUMEXT	ALUMORD	ALUMPROF	TITUL	
ALUMEXT	1.000				
ALUMORD	-0.032	1.000			
ALUMPROF	-0.315	-0.029	1.000		
TITUL	-0.458	-0.132	0.443	1.000	
LOGYP1	-0.152	-0.030	0.160	0.326	
GASTOED	-0.037	0.031	-0.049	-0.191	
DIST	0.072	-0.027	-0.019	-0.113	
PP	-0.031	-0.007	0.042	0.066	
PSOE	0.072	-0.015	-0.080	-0.055	
	LOGYP1	GASTOED	DIST	PP	PSOE
ALUMEXT	LOGYP1	GASTOED	DIST	PP	PSOE
ALUMEXT ALUMORD	LOGYP1	GASTOED	DIST	PP	PSOE
ALUMEXT ALUMORD ALUMPROF	LOGYP1	GASTOED	DIST	PP	PSOE
ALUMEXT ALUMORD ALUMPROF TITUL	LOGYP1	GASTOED	DIST	PP	PSOE
ALUMEXT ALUMORD ALUMPROF TITUL LOGYP1	LOGYP1	GASTOED	DIST	PP	PSOE
ALUMEXT ALUMORD ALUMPROF TITUL LOGYP1 GASTOED	LOGYP1 1.000 -0.152	GASTOED	DIST	PP	PSOE
ALUMEXT ALUMORD ALUMPROF TITUL LOGYP1 GASTOED DIST	1.000 -0.152 -0.127	GASTOED 1.000 0.253	DIST 1.000	PP	PSOE
ALUMEXT ALUMORD ALUMPROF TITUL LOGYP1 GASTOED DIST PP	1.000 -0.152 -0.127 0.317	GASTOED 1.000 0.253 0.103	DIST 1.000 0.322	PP 1.000	PSOE
ALUMEXT ALUMORD ALUMPROF TITUL LOGYP1 GASTOED DIST PP PSOE	LOGYP1 1.000 -0.152 -0.127 0.317 -0.300	GASTOED 1.000 0.253 0.103 -0.183	DIST 1.000 0.322 -0.267	PP 1.000 -0.799	PSOE 1.000

Table 3. Correlation matrix of model regressors

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INNOVATION PROFILES OF SPANISH AUTONOMOUS REGIONS

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KEYWORDS

Innovation quality, Electre Tri, Spanish Autonomous Regions, and Innovation Clustering.

ABSTRACT

The aim of the following article is to study the process of innovation convergence amongst the Spanish Autonomous Regions.

To this end the research has been based on the data analysis from the INE (Spanish National Institute of Statistics) Innovation surveys from 2005 to 2006.

The methodology used will allow us to set up an Autonomous Regions Ranking per year, clustering per groups of innovation quality, so we could analyze the evolution of these rankings to reveal the existence of downward/upward trend changes during the period analyzed in the different Spanish Autonomous Regions.

It will be set out having into consideration all the data and variables offered by the INE at Autonomous Region level on the enterprise technological innovation survey, so it will be analyzed among other variables the intensity of innovation, the number of innovative enterprises and the number of innovative SMEs.

Those classifications will be obtained throughout the application of a non compensatory multicriteria methodology based on outranking relations: Electre Tri method.

INTRODUCTION AND LITERATURE SURVEY

Nowadays Spanish economy belongs to the top ten of the largest worldwide economies, according to the World Bank. Research, development and innovation are the pillars of growth for the most developed economies.

Nevertheless there is a significant gap between the position of Spain in relation to Europe concerning the research, development and innovation, R&D&I.

Spain has been characterized historically to be under the European R&D&I averages, being the main burden on its economy. According Eurostat the percentage of investment on R&D divided by the GDP in Spain and the European Union (25 Countries) has been respectively in 1995 (0.81, 1.84), in 2000 (0.94, 1.88) and in 2005 (1.13, 1.85).

Having into consideration only the 15-EU, fifteen European Union State Members before 1st May 2004, this is the position of Spain, with 1,07%, related to the 15-EU technological effort, id est, percentage of investment on R&D divided by the GDP:



R&D are key factors to increase the economic growth, although the major driver of the economy, increasing productivity, is the innovation, what means a new way of doing something, with revolutionary changes not only in products, but also in processes or even in marketing or organization. Innovation is a critical add value linked to performance and growth improvements in efficiency.

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) Following Staff, Luecke and Katz (2003), innovation is "the successful introduction of a new thing or method . .

. the embodiment, combination, or synthesis of knowledge in original, relevant, valued new products, processes, or services."

Some of the most significant studies about the importance, definition, and differences from innovation and R&D has been carried out by Schumpeter (1934), Dosi (1982), Freeman (1973), von Hippel (1988), Cooke (1997: 2006), Amabile et al. (1996), Cabral (1998, 2003), Mckeown (2008), Luecke and Katz (2003), Thomke (2003), Fagerberg et al. (2004), Fagerberg (2004), Davila et al. (2006), Sarkar (2007).

Not only researchers, but also international organizations have studied the importance of innovation in the economy growth. According to the OECD (2008) innovation is the "creative work undertaken on a systematic basis in order to increase the stock of knowledge, including knowledge of human, culture and society, and the use of this stock of knowledge to devise new applications". European Commission Green Book, 1996, defined innovation as "the adequate production, assimilation and exportation of the newness in the economic and social domains...'

Beyond definitions it must be studied the innovation quantitatively, in order to understand better the contribution of the innovation inputs to the national economies, and the contribution of the different national regions to the national innovation add value to the economy.

In this sense there are internationally three main references that give international standard guidelines in the measurement of the innovation: the Frascati Manual from 1963, the OECD Oslo Manual from 1995, and the OECD Oslo Manual from 2005.

Following the previous suggestions innovation has been worldwide studied throughout the Global Innovation Index. The World Business/INSEAD Global Innovation Index (GII) was conceived at INSEAD as a formal model to help illuminate the degree to which individual nations and regions are currently responding to the challenge of innovation. The last edition has been published in 2009 by Soumitra Dutta.

At European Union level, although the OECD and Cotec Foundation Reports are good data sources, the Statistics EU Agency Eurostat is the most authorized source that measures the evolution of innovation in the EU following the previous manuals. Another very relevant references are the European Innovation Progress Report 2008 and the European innovation scoreboard 2007, both published by the European Commission Inno Policy Trendchart. As well as Spain has historically a deficits in R&D&I activities as compared to Europe, the European Union has as well a historical R&D&I deficit as compared to the United States and Japan. The following graph shows the contribution of business sector to R&D&I expenditure (GERD) in the three main regions of the world.



^{0.9} 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 Source: Working paper on innovation policy in Spain based on the data bases Eurostat and OCDE. CSIC (2003).

The European Union strategic goal for the next decade "of becoming the most competitive and dynamic knowledge-based economy in the world capable of sustainable economic growth with more and better jobs and greater social cohesion" has been set up by the Lisbon European Council in 2000. Within this global objective, the Lisbon Strategy has set as a goal that their average expenditure on R&D should be 3 % of GNP.

At a national level, the Spanish National Institute of Statistic coordinated with the Eurostat, and within the framework of the OECD Oslo Manual and the Frascati Manual, measures the technological Innovation in the Spanish Companies.

The aim of the present work is to analyze the innovation convergence amongst the Spanish Autonomous Regions, clustering them in three different innovation groups.

This study is especially relevant to evaluate the contribution of each Autonomous Region to the growth of the Spanish economy, as well as to the global European Union innovation goal. It has a key importance not only for the previous reasons, but also because clustering the 17 Autonomous Regions in 2005 and 2006 by innovation quality groups, we could analyze its up/downward evolution.

Concerning the previous studies on the Spanish R&D&I framework it is relevant to mention the contribution of Muñoz (1999), who explains that the Spainish autarchy take off was apparently independent of the efforts in R&D&I. How innovation varies from one region to another has been analyzed by Acosta and Coronado (1999) and by Baumert and Heijs (2002).

Sanz-Menéndez (1997) studied the different efforts made in Spain on science and technology policies.

Previous efforts introduced the national scientific community into the international research area.

Quintanilla et al. (1992), Cami et al. (1993; 1997). These innovations had a strong impact on productivity and economic growth. Espinosa de los Monteros et al., 1998; 1999).

The most relevant study about the panoramic of the innovation in Spain through the evolution of regional indicators has been carried out in 2007 by M. Gómez, J.M. Zabala and I. Fernández. In this article it has been studied the evolution of quantitative indicators that are related, directly or indirectly, with the innovation processes and the eminently regional perspective in the presentation of the information.

It is underlined that in spite of the last statistic improvements and more sophisticated indicators, in many occasions there is no enough regional information available, which would be needed for the improvement of the necessary innovation study in Spain.

The Regional System of Innovation studies, such as the Gómez et al. (2008) study and the model that we present in this article, is considered as an useful tool for the study of the economy performance and innovation. Cooke et al. (1997), Doloreux (2002), Doloreux and Parto (2002; 2005). Besides being an important tool to enlarge the understanding of the processes of companies innovation. Asheim and Coenen (2005), Castellaci et al. (2005).

Others interesant researches of innovation at a regional level has been carried out by Braczyk et al. (1996), Howells (1999), Landabaso et al. (1999), Morgan and Nauwelaers (1999) and Koschatsky et al. (2000)

They are multiple studies that have approached to the measurement of the innovative capacity of the territories either on national, regional, or local level, such as Furman et al. (2002), Archibugi and Coco (2004), Faber and Hesen (2004), Zabala-Iturriagagoitia et al. (2008). That is why one of the main focuses of attention within the related bibliography is linked with the development of the most suitable innovation analysis systems and indicators, such as the Manual of Oslo (2005), Manual of Frascati (1994), Den Hertog et al. (1995) or Leydesdorff (2001).

It has been carried out a very significant study about the regional systems of innovation and the knowledge production function with special emphasis on the Spanish case by M. Buesa et al. (2006). It is analyzed the Spanish R&D system throughout a multivariate data analysis. Most outstanding contribution is the identification and analysis of four factors that have an enormous influence in the regional innovation evolution. These factors are: 1. Regional and productive environment for innovation, 2. Role of Universities, 3.

Role of the civil service, and 4. Role of innovating firms.

The organization of the process of innovation in the Spanish companies has been analyzed by J. Galende (2008). He concludes his research explaining that the generation of innovation is mainly based on internal activities, especially those activities of R&D (fundamentally technological development), being nowadays the external acquisition a marginal method.

During the Franco dictatorship the technology and the science worsened considerably due to diverse causes, to highlight mainly, the international isolation to which was subjected the country, what was difficult to overcome.

During this time the technological progress and scientists met one of his more negative stages. On the other hand the creation of the Superior Council of Scientific Investigations (CSIC) didn't suppose the increase of innovation on the Spanish economy.

On democracy it has been set up the Center for the Technological and Industrial Development (CDTI), as it has been published the Law of university reform and the general Law of development of the scientific activity and the technological development, as well as the National Plans for R&D.

In 1979 innovation efforts were pointed out in the political agenda of the Socialist Party (PSOE), including in their program the political goal of increasing the "public resources devoted to R&D activities, with the hope to drive also an increase in the research and innovation efforts of the private sector.", as it has been since 1979 included promotion of innovation in Spain in all the agendas of the democratic governments.

After Spanish Constitution of 1978 Spain is composed of 17 Autonomous Regions; Galicia, Navarre, Madrid, La Rioja, Aragon, Catalonia, Valencia, Castile-La Mancha, Extremadura, Castile and León, Asturias, Cantabria, Basque Country, Murcia, Andalusia, Balearic Islands and Canary Islands, plus two autonomous cities; Ceuta and Melilla.

As there are relevant heterogeneities and divergences between the regions in Spain, the Spanish National Institute of Statistic assesses (last definitive data published for 2006 in December 2008) the innovation index in each Autonomous Region, using the following set of eight variables that we decided to include in our model as it is firstly the most authorized innovation data source in Spain, and secondly because it has published a complete and specific survey that provides information on the structure of the innovation processes of companies:

- 1. Innovative companies: Innovative companies on the total of companies in the Autonomous Regions in 2005.
- 2. EIN Companies: Innovative companies or with innovations in course or not successful innovations on the total of companies in the Autonomous Regions in 2005.
- 3. Product innovative companies: Innovative companies in product during the period 2003-2005 regarding the total amount of innovative companies in that period.
- 4. Process innovative companies: Innovative companies in processes during the period 2003-2005 regarding the total amount of innovative companies in that period.
- 5. Product and process innovative companies: Innovative companies in product and processes during the period 2003-2005 regarding the total amount of innovative companies in that period.
- 6. Innovation expenses in less 250 employees: Expense percentage in innovative activities of the companies of less than 250 employees regarding the total expense in innovation.
- 7. Innovation expenses in 250 employees or more: Expense percentage in innovative activities of the companies with 250 or more employees regarding the total expense in innovation.
- 8. Intensity of the innovation: ((Expenses in innovation / figure of business) x 100).

Among all the Spanish Autonomous Regions, there are four of them above the national average: Madrid, Catalonia, Navarre and Basque Country. Gómez et al. (2008).

The concentration of R&D&I capabilities in Madrid and Catalonia has been historically the main characteristic of the R&D&I Spanish system. Muñoz et al. (2000). For instance, in 1997 Madrid represented the 33% of the Spanish GERD, Catalonia the 21% and the Basque Country the 9%, whilst eleven less developed regions represented only the 32%. INE (1999).

Although Moso and Olazarán (2001) estimated that Catalonia and Basque Country lead the R&D&I in Spain, whilst Madrid is at the average R&D&I level, having into consideration previous studies that make comparison between the Spanish Autonomous Regions, including together R&D&I, we could conclude a priory that there is a huge gap in innovation between Madrid-Catalonia and all the others regions.

Nevertheless we consider that this is a very complex topic of study, not only because many different determinants have a considerable influence in the innovation performance, but also because it must be analyzed the innovation separately from the R&D.

METHODOLOGY

We have analyzed data from the INE Innovation surveys of 2005 and 2006 (2007 data are not definitive yet) to obtain classifications of Spanish Regions into three groups: very innovative regions, average level innovative regions and lower level innovative regions.

To achieve this goal we have worked with a non compensatory, outranking relations based method: Electre Tri. This Electre Tri method has been applied to the result of a principal component analysis (PCA) carried out over the whole set of variables.

More specifically, we have done a principal component analysis over the eight variables taken into account, as a result we have obtain two factors. Then we have used Electre Tri to classify the regions into the three categories described above.

Electre Tri is a multicriteria decision aid method and thanks to it we are going to decide where regions have to be classified into predefined categories. Electre TRI deals with the issue relating to classifying each alternative into a pre-defined category.

Reference alternatives are used to segment criteria into categories: each category is limited below and above by two reference alternatives and each reference alternative thus serves as a border for the two categories, one upper and the other lower.

Electre TRI is therefore a method of assigning action (regions) to pre-defined categories (hypothetical reference regions). The assigning of an action (region) "a" results from the comparing of "a" to the profiles (action – regions- reference) that define the limits of categories.

To apply Electre Tri to our data we are considering that factors obtained from PCA are criteria and regions are alternatives. Importance parameters for the criteria will be the percentage of variance explained by each factor.

CLUSTERING THE SPANISH AUTONOMOUS REGIONS IN FOUR STEPS

In a first step we have done a principal component analysis over the eight variables taken into account to reduce the dimension of the problem and to obtain what will be the future weights of criteria in Electre Tri. As a result we have obtained two factors.

It exists, so much in the year 2005 as in 2006, two critical dimensions when measuring the innovation: Firstly what we'll call "innovative companies". In this factor we find high and positive correlations in the following variables: innovative companies (0,985 in 2005 and 0.980 in 2006), EIN Companies (0.988 in 2005 and 0.992 in 2006), Product innovative companies

(0.986 in 2005 and 0.994 in 2006), Process innovative companies and Product and process innovative companies (0.986 in 2005 and 0.983 in 2006). Secondly, what we will call "Expenses in innovation", which is negatively correlated with the expenses percentage in innovation in companies of less than 250 employees (-0.933 in 2005 and -0.917 in 2006), and positively correlated with the Expense percentage in innovative activities of the companies with 250 or more employees (0.933 in 2005 and 0.917 in 2006) and the Intensity of the innovation (0.643 in 2005 and 0.579 in 2006)

These two factors or dimensions explain, in 2005 90,417% of the total variance, and 89,469% in 2006.

Explained total variance in 2005			
		Initial eigen	values
Component	Total	Variance	Accumulated
	Total	Percentage	%
1	5,387	67,431	67,341
2	1,846	23,076	90,417
3	0,745	9,308	99,725
4	0,018	0,223	99,948
5	0,004	0,048	99,996
6	0,000	0,004	100,000
7	2,222	2 777E 0	100.000
/	E-10	2,///E-9	100,000
8	5,139	6.424E-16	100.000
0	E-17	0,4240-10	100,000

Extraction method: Principal Component Analysis.

Explained total variance in 2006				
		Initial eigen	values	
Component	Total	Variance	Accumulated	
	Total	Percentage	%	
1	5,440	68,004	68,004	
2	1,717	21,466	89,469	
3	0,821	10,268	99,737	
4	0,011	0,143	99,880	
5	0,006	0,076	99,956	
6	0,003	0,044	99,999	
7	5,043	0.001	100,000	
/	E-5	0,001		
Q	1,281	1 601E 0	100,000	
0	E-10	1,001E-9		

Extraction method: : Principal Component Analysis..

It could be interesting to compare two univariate rankings: those of the factors obtained above. That means to compare the ranking based on the number of innovative companies (including, EIN companies, product or process innovative companies and product and process innovative companies) with the expenses in innovation (factor two). This comparison gives us idea of how different are the results depending the variables used to build a ranking.

Autonomous Regions ranking in 2005				
Ranking according to Ranking according to the				
the " innovative	"expenses in innovation":			

companies": Factor	Factor Two
one	
Catalonia	Aragón
Madrid	Galicia
Valencia	Castile and León
Andalusia	Madrid
Basque Country	Basque Country
Canary Islands	Catalonia
Murcia	Asturias
Galicia	Navarre
Castile - La Mancha	Castile - La Mancha
Castile and León	Andalusia
Balearic Islands	Cantabria
Extremadura	Murcia
Cantabria	Extremadura
La Rioja	La Rioja
Navarre	Valencia
Asturias	Canary Islands
Aragón	Balearic Islands

Autonomous Regions ranking in 2006			
Ranking according to the "innovative companies": Factor one	Ranking according to the "expenses in innovation": Factor Two		
Catalonia	Asturias		
Madrid	Aragón		
Andalusia	Galicia		
Valencia	Madrid		
Basque Country	Basque Country		
Murcia	Castile and León		
Canary Islands	Navarre		
Castile- La Mancha	Catalonia		
Galicia	Extremadura		
Castile and León	Andalusia		
Balearic Islands	Castile La Mancha		
Cantabria	Murcia		
Aragon	Cantabria		
Extremadura	Cantabria		
Navarre	La Rioja		
La Rioja	Balearic Islands		
Asturias	Valencia		

Because of the results showed above we will to set up a classification of Autonomous Regions having into consideration all the variables, resumed in the two factors obtained form Principal Component Analysis. To do that we have used the multicriteria decision method Electre Tri. In our study, to apply Electre Tri, criteria will be the two factors, the weight of each factor will be the variance explained by the factor and alternatives will be Autonomous Regions. Autonomous Regions have been classified in three predefined groups according to their innovative profile: very innovative regions, average level innovative regions and lower innovative level regions.

The results of the Electre Tri classifications for 2005 and 2006 are shown below:

Autonomous Regions innovation cluster in 2005 using all variables			
	Pessimistic	Optimistic	
	Classification	Classification	
Very innovative Autonomous Regions	Madrid Basque Country	Andalusia Aragón Castile and León Catalonia Valencia Galicia Madrid Basque Country	
Average level innovative Autonomous Regions	Andalusia Castile and León Castile and La Mancha Catalonia Galicia Murcia	Asturias Balearic Islands Canary Islands Cantabria Castile and la Mancha Extremadura Murcia Navarre	
Lower innovative level Autonomous Regions	Aragón Asturias Balearic Islands Canary Islands Cantabria Valencia Extremadura Navarre Bioja	Rioja	

Autonomous Regions innovation cluster in 2006 using all variables			
	Pessimistic	Optimistic Classification	
Very innovative Autonomous Regions	Madrid Basque Country	Andalusia Aragón Asturias Castile and León Catalonia Valencia Galicia Madrid Murcia Basque Country	
Average level innovative Autonomous Regions	Andalusia Castille and León Castile and la Mancha Catalonia Galicia	Balearic Islands Canary Islands Castile la Mancha Extremadura Navarre	
Lower	Aragón	Cantabria	

innovative	Asturias	Rioja
level	Balearic Islands	
Autonomous	Canary Islands	
Regions	Cantabria	
	Valencia	
	Extremadura	
	Murcia	
	Navarra	
	Rioja	

The final cluster of Autonomous Regions shows a pessimistic and optimistic classification in both years 2005 and 2006 within three predefined cluster groups of innovation quality. As it can be observed both classifications don't match up, which is normal. The usual way to proceed in such cases is to retain the pessimistic classification. Note that Autonomous Regions classified in the same category both in the pessimistic and optimistic classifications are Autonomous Regions with a robust classification (Madrid and Basque Country for example)

So the reader could observe by himself the upward/downward evolution of each Autonomous Region, which reveals the existence of innovation trend changes during the period analyzed in the different Spanish Autonomous Regions.

Final cluster agree with the previous studies and shows at the same time very interesting new information about the innovation evolution in the Spanish Autonomous Regions.

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INNOVATION EFFICIENCY IN SPAIN: AN ANALYSIS BY ACTIVITY BRANCH.

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KEYWORDS

Productivity, Electre Tri, Innovation, Spanish Economy, Activity Branches, and Data Envelopment Analysis.

ABSTRACT

The increase in productivity is an obvious objective for business, moreover with the research and development objectives set out for Barcelona 2010 and the Lisbon Summit. Productivity is linked to efficiency as enterprises have increased productivity when they need less input to achieve certain outputs or when they increase outputs with the same inputs.

The objective for this article is to analyze the innovation efficiency in Spain by activity branch. To this end we will work with the 2006 data from the INE (Spanish National Institute of Statistics) innovation and R&D activities surveys. To this aim, we will use the following methodology for the efficiency analysis: the one based on output oriented DEA (Data Envelopment Analysis) with constant returns to scale.

This technique will be completed in two aspects. Firstly with the introduction of more inputs and outputs without causing an increment of efficient units and, secondly the study will be completed with a robust analysis to improve the DEA discrimination capacity.

MOTIVATION OF THE RESEARCH AND LITERATURE SURVEY

The structure of the Spanish economy is suffering nowadays some very significant changes marked by a double crisis at the same time. On one hand the serious international crisis, and on the other hand a national crisis product of a long term growth model based on exhausted activity branches.

It has been pointed out within the new strategic goals for the next decade set at the Lisbon European Council, in march 2000, that the European Union will become the most competitive and dynamic knowledge-based economy in the world, capable of sustainable economic growth with more and better jobs and greater social cohesion. Achieving these goals requires an overall strategy aimed at preparing the transition to a knowledge-based economy and society by better policies for the information society and R&D, as well as by stepping up the process of structural reform for competitiveness and innovation and by completing the internal market. (Lisbon European Council, 2000).

Spain, as a Member State of the European Union, should add value to the Union to become the most competitive, efficient, and dynamic economy in the world based on the knowledge, such as education, innovation, research and development.

In that point the following questions arises:

- Which the strengths and weaknesses of the Spanish economy are?
- In what economic activities should Spain specialize?
- Which is the role of the innovation in the transformation of the economic structure of Spain?
- Which is the efficiency in the innovation of the different branches of activity of the Spanish economy?
- In which branches is obtained the bigger productivity of the investments?
- Which activity branches of the Spanish economy are the most efficient ones?

All these key questions will be studied throughout the present paper to understand the current structure of the Spanish economy and to be able to offer information to economic politics decision makers.

Structural transformations needed to the economic growth and increase of the rent per capita imply changes of certain relevance in the structure of the production, in the role of the trade and in the public sector weight. (García and Myro, 2008).

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) These changes leaded by the upward tendency of some activity branches and the decline of others, alter the structure of the whole economy. The research, development and innovation, all of them focused on the increase of productivity, are needed to lead these significant structure changes. Throughout the base of a balanced and sustainable economic growth based on innovation must be designed the nowadays Spanish economy structure change.

We conclude that the first motivation of this paper is to answer all the previous key questions related to the Spanish economy, but the second motivation is the methodological one, because methodologically it has never been applied such a innovative technique to try to answer to the previous questions.

Although there has been carried out very interesting researches on this topic (Buesa *et al*, 2006), (Galende del Canto 2008), (Gómez and Zabala 2008) it has not been applied the methodologically solution to the problem offered in this paper even by the most advanced DEA research methods. (Cooper *et al*. 2004), (Doyle and Green, 1994), (Dyson *et al*, 2001), (Lugones *et al*, 2003), (Madlener *et al*, 2006), (Maystre *et al*, 1994), (Raftery, 1993), (Roy and Bouyssou, 1993), (Zhu and Cook, 2007).

In order to follow the most authorized data analysis methodology it has been developed the study under the Oslo Manual framework and in concordance with the the INNO-policy reports, INNO Metrics (2007) and the European regional innovation scoreboard report (2006).

METHODOLOGY

The objective for this article is to analyze the innovation efficiency in Spain by activity branch. To this end we will work with the 2006 data from the Spanish National Institute of Statistics innovation and R&D activities surveys.

To this aim, we will use the following methodology for the efficiency analysis: the one based on output oriented DEA (Data Envelopment Analysis) with constant returns to scale and without a priori information about weights.

DEA allows each decision making unit (DMU, branches in our study) to specify its own weights so as to obtain a maximum efficiency score for itself.

Without the possibility of introducing weight restrictions, complete weight flexibility is allowed. This may result in identifying a Decision Making Unit (DMU) with an unrealistic weighting behavior to be efficient. Problems arising from the total flexibility of weights in DEA model are often dealt incorporating weight restrictions. Nevertheless, weight restrictions must be meaningful and justified. Consequently, this poses a new problem to the analyst who should be able to explain why particular weights restrictions were used, especially when there is no full cooperation with the stakeholders or there is a lack of information.

Moreover, weight restrictions can pose as well technical and computational problems in some cases. For example, it is necessary to look for a compromise unique weight bounds suitable for all the units.

Due to these problems, we propose to take a different approach. We are going to proceed in two steps. Firstly, we are going to use cross efficiency analysis to take into account the whole set of weights families to lead each DMU (branches) to reach its maximum efficiency (to appear under the "best possible light"). And secondly, we will use Multicriteria Decision Aid to increase the discrimant power of DEA for the efficient branches.

The multicriteria Decision Aid method chosen will be Electre Tri. Electre Tri is a non compensatory, outranking relations based method and deals with the issue relating to classifying each alternative into a predefined category. Reference alternatives are used to segment criteria into categories: each category is limited below and above by two reference alternatives and each reference alternative thus serves as a border for the two categories, one upper and the other one lower.

Electre Tri is therefore a method of assigning action (regions) to pre-defined categories (hypothetical reference regions). The assigning of an action (region) "a" results from the comparing of "a" to the profiles (action – regions- reference) that define the limits of categories. Electre Tri will be applied to the cross-efficiency matrix of the DEA-efficient DMUs/branches.

Branches will be classified into two groups: those branches that are efficient or reach good enough efficiency values over the different set of weights for DMUs, and those ones that are efficient with their optimal weights but that reach bad efficiency values with the rest of weights for the others DMUs. We could also name these classes as the robust efficient branches and the non robust efficient branches.

As a prior step to DEA analysis we will do Principal Components Analysis (PCA) over the set of inputs and, separately, over the set of outputs. This is done due to other of the pitfalls of DEA: when there are many inputs and outputs the number of efficient DMUs increases. In our case if we apply DEA directly to the original set of inputs and outputs all the branches will be efficient.

The result of the study of the efficiency on the activity branches using the total of the original variables indicates that all the activity branches are efficient. For that reason it is necessary to carry out the study of the analysis of efficiency on the main components of the inputs on one hand and of the outputs on the other hand.

This identification of the most innovative efficiency Spanish economy activity branches will be carried out in three steps:

- 1. Firstly we will obtain the principal components of the inputs and, separately, of the outputs.
- 2. Secondly it will be identified the efficient and the non efficient activity branches obtained by a output oriented DEA applied over the principal components of the inputs and of the outputs.
- **3.** Thirdly it will be improved the capacity of discrimination of the previous DEA by carrying out an Electre Tri over the cross-efficiency matrix of the efficient activity branches where all the criteria have equal weights. This Electre Tri will create two groups within the efficient activity branches, being fifteen efficient activity branches in the first group and eleven efficient activity branches in the second group.

ACTIVITY BRANCHES OF THE SPANISH ECONOMY

First of all it must be introduced the activity branches in which of research is focused on. How to separate or distinguish the different activity branches from the whole economy it is itself an interesting topic of research.

We follow the international main stream activity branches division, leaded by the OECD Oslo Manual from 1995, improved in 2005. This reference gives the main international standard guidelines, followed as well by the INE (Spanish national institute of statistic).

Last data published about the Spanish activity branches, following the previous methodology, has been published by the INE in 2006 within its technological innovation in the companies in 2006 organized per activity branches and offering main indicators of technological innovation in 2006.

One of the most interesting information offered is the innovation intensity of each activity branch, what means the total expenses in innovation related to the total figure of business. On the next paragraphs the different Spanish economy activity branches are enumerated, and at the same time the percentages of its innovation intensity are showed. All the activity branches has been ordered decreasingly, so it is possible not only to know which one has a bigger percentage of expenses in innovation, but also to understand how efficient these expenses are by checking the further table that classifies activity branches in order to their efficiency.

Obviously the research and development services activity branch leads this ranking, with an outstanding percentages of innovation intensity of 106,59%, followed, with a huge gap behind, by the aerospace activity branch, which has a 24,53% of innovation intensity. As it could be checked later on, both of the previous sectors are efficient.

Nevertheless a significant percentage of innovation intensity doesn't mean to be efficient, as it happens in the pharmacy activity branch, with a 5,11% of innovation intensity and with an under average efficiency level (it will be shown later).

Mail and telecommunications had in 2006 a 3,67% of innovation intensity, optics instruments and watchmaking 3,15%, office, calculation and computer machines 3,12%, electronic components 2,76%, another material of transport 2,53%, automobiles 2,39%, radio, TV and communication devices 2,34%, naval 2,27%, computer programs 1,76%, machinery and mechanical machines 1,65%, edition, impression and reproduction 1,58%, electric machines 1,56%, another manufactures 1,52%, transport and storage 1,40%, chemistry (except pharmacy) 1,34%, metallica

manufactures 1,22%, textile 1,19%, rubber and plastic 1,13, other computer activities 1,10%, cardboard and paper 1,08, non metallic minerals 0,93%,

recycled 0,88%, services to companies 0,85%, agriculture 0,80%, furniture 0,80%, leather and footwear 0,74%, feeding, drinks and tobacco

0,71%, wood and cork (except furniture) 0,71%, public, social and collective services 0,68%, strong metals

0,65%, extractive 0,63%, making and furrier 0,50%, electricity, gas and water 0,50%, non strong metals 0,47%, financial services 0,31%, construction 0,22%, coke, petroleum and nuclear fuel 0,13%, and trade and hostelry 0,13% respectively.

CORE VARIABLES TO ANALYZE THE INNOVATIVE EFFICIENCY

The set of variables used in our model are divided in two groups: the input and the outputs variables. The available variables that explains better the innovative efficiency input per activity branch in 2006 are:

- Total of innovative companies.
- Expenses in innovation: total in thousands of Euros.
- Expenses in innovation: R&D (internal and external) (%).
- Expenses in innovation: other innovative activities (%).
- Percentage of companies with innovative activities in 2006 over the total number of companies.

- Percentage of companies with innovative activities with internal R&D.
- Percentage of companies with innovative activities with external acquisition of R&D.
- Percentage of companies with innovative activities with acquisition of machinery, tools and software.
- Percentage of companies with innovative activities with acquisition of external knowledge.
- Percentage of companies with formative innovative activities.
- Percentage of companies with innovative activities with introduction of innovation in the market.
- Percentage of companies with innovative activities in design and other applications to production and/or distribution.

On the other hand the available variables that explains better the innovative efficiency input per activity branch in 2006 are:

- Intensity of innovation of the total companies.
- Intensity of innovation of the companies with innovation activities.
- Intensity of innovation of the companies with R&D activities.
- Percentage of companies with innovation in product (improvement of goods or services).
- Percentage of companies with innovation in the processes.
- Percentage of companies with innovation in product and processes.
- Percentage of companies that have introduced products that were a novelty only for the company.
- Percentage of companies that have introduced products that were a novelty for the market.
- Percentage of the company figure of business in 2006 consequence of the goods and/or services that were a novelty only for the company.
- Percentage of the company figure of business in 2006 consequence of the goods and/or services that were a novelty for the market.
- Percentage of the company figure of business in 2006 consequence of the goods and/or services that were a novelty only for the company in companies with innovations in course or not successful.
- Percentage of the company figure of business in 2006 consequence of the goods and/or services that were a novelty for the market in companies with innovations in course or not successful.

IDENTIFICATION OF THE MOST INNOVATIVE EFFICIENCY SPANISH ECONOMY ACTIVITY BRANCHES IN THREE STEPS

As developing the analysis having into consideration the total variables gives as result that all the activity branches are efficient, it has been necessary to improve the method by carring out the efficiency analysis over the principal components of the inputs and outputs.

First step:

Firstly we will obtain the principal components of the inputs and, separately, of the outputs.

We begin with the results for the inputs. It has been identified four main factors over the inputs, which have a global variance explanation power of 80,902%. The explained variance of each component in 2006 could be observed in the following table.

Explained total variance: inputs				
Component	Total	Variance Percentage	Accumulated %	
1	5,639	31,257	31,257	
2	1,582	19,883	51,140	
3	1,379	17,112	68,251	
4	1,109	12,650	80,902	
5	0,782			
6	0,480			
7	0,389			
8	0,275			
9	0,236			
10	0,093			
11	0,037			
12	1,20E-016			

Extraction method: Principal Component Analysis.

Once applied the matrix of rotated component weights, using the rotated method of Varimax normalization with Kaiser, it has been obtained four main factors that explains the most of the variance and oppose some variables to anothers.

The first factor explains the 31,257% of the whole variance. It oppose the "Expenses in innovation: R&D (internal and external) (%)" with a correlation value of 0,928, the "Percentage of companies with innovative activities in 2006 over the total number of companies" with a correlation of 0,545, the "Percentage of companies with innovative activities with internal R&D" with a correlation of 0,629, to the "Expenses in innovation: other innovative activities (%)", with a negative correlation of 0,928, the "Percentage of companies with innovative activities with acquisition of machinery, tools and software", with a negative correlation of 0,793.

The second factor explains the 19,883% of the whole variance. It oppose the "Total of innovative companies", with a negative correlation of 0,865 to "Percentage of companies with innovative activities

with introduction of innovation in the market", with a correlation of 0,678 and "Percentage of companies with innovative activities in design and other applications to production and/or distribution", with a correlation of 0,518.

The third factor explains the 17,112% of the whole variance. It includes the "Percentage of companies with innovative activities with external acquisition of R&D", with a correlation of 0,773, and the "Percentage of companies with innovative activities with acquisition of external knowledge" with a correlation of 0,941%.

The fourth factor explains the 12,650% of the whole variance. It includes the "Expenses in innovation: total in thousands of Euros" with a correlation of 0,894, and the "Percentage of companies with formative innovative activities", with a correlation of 0,530.

We move now to the results for the outputs. It has been identified as well four main factors over the outputs, which have bigger global variance explanation power. All the four factors explain the 92,686% of the variance. The explained variance of each component in 2006 could be observed in the following table.

Explained total variance: outputs				
Component	nent Total Variance Percentage 5,903 35,489		Accumulated % 35,489	
1				
2	2,727	27,430	62,919	
3	1,325	17,282	80,202	
4	1,167	12,484	92,686	
5	0,615			
6	0,163			
7	0,047			
8	0,032			
9	0,013			
10	0,006			
11	0,001			
12	0.001			

Extraction method: Principal Component Analysis.

As it has been previously done in the inputs case, here it has been as well applied the matrix of rotated component weights, using the rotated method of Varimax normalization with Kaiser, and it has been obtained four main factors that explains the most of the variance and oppose some variables to anothers.

The first factor explains the 35,489% of the whole variance. It includes the "Intensity of innovation of the total companies", with a correlation of 0,954%,, the "Intensity of innovation of the companies with innovation activities" with a correlation of 0,951%, the "Intensity of innovation of the companies with R&D activities" with a correlation of 0,945%, the "Percentage of the company figure of business in 2006 consequence of the goods and/or services that were a novelty for the market" with a correlation of 0,827%, and the "Percentage of the company figure of business in 2006 consequence of the goods and/or services that were a

novelty for the market in companies with innovations in course or not successful" with a correlation of 0,802%.

The second factor explains the 27,430% of the whole variance. It includes the "Percentage of companies that have introduced products that were a novelty for the market", with a value of 0,865%, the "Percentage of companies with innovation in product (improvement of goods or services)" with a correlation of 0,833%, and the "Percentage of companies that have introduced products that were a novelty only for the company" with a correlation of 0,793%.

The third factor explains the 17,282% of the whole variance. It includes the "Percentage of the company figure of business in 2006 consequence of the goods and/or services that were a novelty only for the company in companies with innovations in course or not successful", with a correlation of 0,925, and the "Percentage of the company figure of business in 2006 consequence of the goods and/or services that were a novelty only for the company figure of business in 2006 consequence of the goods and/or services that were a novelty only for the company", with a correlation of 0,920.

The fourth factor explains the 12,484 of the whole variance. It is directly linked with the "Percentage of companies with innovation in the processes" and has a negative correlation of 0.960, so it explains the percentage of enterprises with a lower processes innovation.

Second step:

Secondly it has been identified the efficient activity branches obtained by a oriented outputs DEA over the principal components of the inputs and of the outputs. By using this technique it is possible to identify which activity branches are efficient and which one aren't. The following table shows the activity branches which are no efficient and indicates the differences in efficiency throughout its percentages:

ACTIVITY BRANCH	Efficiency
Chemistry (except pharmacy)	98,23
Optics instruments and watch-making	97,36
Rubber and plastic	96,57
Machinery and mechanical machines	94,97
Public, social and collective services	94,48
Radio, TV and communication devices	94,25
Wood and cork (except furniture)	93,52
Non metallic minerals	93,1
Furniture	90,83
Phamacy	87,73
Financial Services	84,58
Metallica manufactures	78,86
Trade and hostelry	77,96
Extractive	76,22
Services to companies	75,03
Electricity, gas and water	68.23

By contrast the following table shows all the efficient activity branches having into account both inputs and outputs principal components:

ACTIVITY BRANCH	Efficiency
Making and furrier	100
Textile	100
Agriculture	100
Transport and storage	100
Leather and footwear	100
Edition, impression and reproduction	100
R&D Services	100
Mail and telecommunications	100
Cardboard and paper	100
Another manufactures	100
Naval	100
Feeding, drinks and tobacco	100
Other computer activities	100
Construction	100
Automobiles	100
Strong metals	100
Coke, petroleum and nuclear fuel	100
Electric machines	100
Electronic components	100
Non strong metals	100
Recycled	100
Office, calculation and computer machines	100
Another material of transport	100
Computer programs	100
Aerospace	100
Electric machines	100

Third step:

Once the previous analysis has been carried out, the final and most significance add value of this research has been completed by improving the capacity of discrimination of the DEA method by carrying out Electre Tri over the cross-efficiency matrix of the efficient activity branches where all the criteria have equal weight. Results are the following:

First class group of efficient activity branches (robust efficient activity branches):

- Edition, impression and reproduction
- Mail and telecommunications
- Cardboard and paper
- Another manufactures
- Feeding, drinks and tobacco
- Automobiles
- Coke, petroleum and nuclear fuel
- Electric machines
- Electronic components
- Non strong metals
- Recycled
- Office, calculation and computer machines
- Another material of transport
- Aerospace
- Electric machines.

Second class group of efficient y activity branches (non robust efficient activity branches):

• Making and furrier

- Textile
- Agriculture
- Transport and storage
- Leather and footwear
- R&D Services
- Naval
- Other computer activities
- Construction
- Strong metals
- Computer programs

This Electre Tri created the two groups within the efficient activity branches showed above, being fifteen efficient activity branches within the first group, what means that these activity branches are not only efficient when the optimal weights for this activity branch has been assigned, but with most of the weights consired for the other activity branches. And the eleven efficient activity branches in the second group belongs to a second category because in that case they are no robust enough as they are only efficient with favorable weights.

CONCLUSIONS

As it has been explained the three main conclusions obtained in this paper are:

- 1. Methodologically it is possible to improve the DEA method by using the Electre Tri over the cross efficiency matrix of the efficient activity branches
- 2. To obtain a more realistic classification than the previous of the Spanish economy activity branches according to their efficiency.
- 3. To be able to classify the efficiency activity branches in three levels: non efficient activity branches, non robust efficient activity branches and robust efficient activity branches

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MODELING THE RELATIONSHIP BETWEEN INDUSTRIAL EMPLOYMENT AND INFORMATION AND COMMUNICATION TECHNOLOGIES

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KEYWORDS

Employment, Modeling Information, Communication, Technologies, Structural equations, SEM.

ABSTRACT

In this paper, we develop a model to measure the effects of Information and Communication Technologies (ICT) on the labor market, aiming to settle down its net effect on employment creation. The main findings are:

1) Related with the sector services, where the regions with worse evolution of the industrial employment showed growth in the *information society* sector services, being it intensive in technology, and a certain negative incidence employment growth in the sector services in general and in the industrial one,

2) Related with the ICT, where two variables have a negative effect on the employment growth: the extranet and the own wireless net. This negative incidence has its base on the positive relationship between productivity and technology. This way, the ICT integration into the industry causes smaller new workers needs.

3) A second group of estimates highlights some of the factors that have influenced the recent industry evolution. The most prominent effect is the incidence of the ICT on the added value. The regions where there is more penetration of the ICT are the ones having bigger industry relevance in the Spanish economy.

4) In addition, the difficulties to find ICT skilled workers specialist is a factor that hinders the added value growth. These results reveal the need of a public policy favoring the skilled labor and the company's technological advances. The conjunction of both factors will improve the industry long-term benefits.

5) A last effects group reveals that regions with bigger industrial production growth have also a bigger growth of the employment in the services sector.

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INTRODUCTION

Technological innovations and employment

The relationship between technology and work is an important, old and controversial field of discussion in the economic and social analysis. In the academic literature, two big tendencies coexist. The first one, the so-called compensation theory, states the positive and long-term influence of technological change on employment. The second, affirms that the technological change weakens, or even eliminates, the positive relationship between technology and number of jobs. Several investigations -e.g. OECD, 1998- show clearly that the technological progress is associated to a high occupation growth, mainly of the skilled labor. Nevertheless, when tying to verify if the most innovative organizations are also the ones creating more employment, must be kept in mind the effects on their rival companies: maybe the innovative firms do create employment but at the cost of destroying it in less competitive rivals.

Overall, the effect of the technological change on employment is the combined result of innovations in productive sectors, of the labor markets (internal and external) existing conditions and of the economic activity institutional frame. When a knowledge intensive company introduces an innovation that increases its labor force, the effects spread to other sectors. The lost jobs due to the technological change tend to take place in the manufacturing sector and among the less skilled workers, while the new ones require more and different skills and concentrate on the services sector. The final effect will be positive if the necessarv conditions are fulfilled. mainly macroeconomic stability and macroeconomic efficiency, besides others relative to the adjustment to the labor market changes and the adaptation of the institutions influencing it.

Besides, there are forces that, spontaneously, could compensate the short-term occupation reduction, resulting from the technical change. These

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) compensatory mechanisms can be clustered (Vivarelli and Pianta, 2000) into six big types; compensation by means of: a) new jobs in other sectors, b) price reduction, c) new investments, d) fall of wages, d) rent increase and f) new products.

Summarizing, the real effect of the technology on the skills, organization and results at employment depends on the labor force characteristics, its learning abilities and experience, organizational structure, human resources management, company interaction with its environment, and on the pattern of economic and social competitiveness. So that, the effect of the technology can only be understood considering (Torrent, 2008) its interaction with the variables mentioned and in relation with the economic and social system in which is applied.

Employment and Information and Communication Technologies

When studying the influence of the ICT on employment creation and destruction is necessary considering, at least conceptually, to improve its understanding three types of effects: direct, indirect and on the markets structure.

a) **Direct effects**: creation of new employments intended for the new products and services that had not been possible without the new technology. b) **Indirect Effects**: the ones derived from their use in any other sector of the economy. The incorporation of a new and more efficient technology generates a substitution of the less efficient technologies used so far. The question is how many employments do they preserve and create or wipe out the ICT, when making more competitive the sectors where they are applied? c) **Effects on market structure** of qualitative and quantitative nature, that influence the type of employment on demand, the skills required and even the labor market configuration.

The above-mentioned factors outline the complexity of the ICT influence in the labor market, and therefore of its evaluation. Being its effects of reinforcement as well as inhibitors, its net effect estimate on employment is not of easy determination. Besides, these effects are non homogeneous neither in all the societies nor in all the economic sectors; depending on the degree the economy of a country or region is able to take advantage of the potential possibilities of the new technologies, in relation with other competitor economies. In addition, it is to consider not only its effect on the number of employments but also on the type jobs, its quality, and wages.

This paper contributes to the evaluation of the ICT effects on the work market, aiming to settle down if its net effects, direct and indirect, on the employment creation are positive or negative. In the next sections, we present the data and method, later a model of structural equations (graph 2) is developed whose parameters are estimated by the method of maximum

likelihood with full information (FIML). The paper finishes with some conclusions and recommendations.

Data and Model

The main statistical source to analyze the industrial employment evolution in Spain is the Industrial Survey, carried out yearly by the National Institute of Statistic (INE). It will also be used the survey of ICT use and electronic trade in the companies, that contains information on the use of the new technologies and their regional diffusion degree. Lastly, the regional accounting and the central directory of companies (DIRCE) complete the information, with data generated by industry, market size and number of companies in each region. All these surveys are representative at regional level.

With regard to time, we consider two types of variables. On one hand, the ones describing time variations (for example, variation of the employment) and, on the other, the ones referred to a year period, having a structural character (for example, number of companies). In the first case, the temporary period is 1996-2006, both included, in the second the year 2006.

The variables considered in modeling the industrial employment behavior are in the chart 1, following.

Name	Label
EM2006	Industry employment (number of workers year 2006)
HT2006	Number of worked hours
NEMP	Number of industry firms
HrelESP	Ratio worked hours in region and nation total (percent)
EMPrel	Ratio number of regional firms to the total nation total (percent)
R_HT_EMP	Worked hours per firm
EMP_DIRC_SC	Ratio variables hrelesp/emprel
E_TIC	Percentage of firms employing, in January 2007, skilled ICT workers
ESP_TIC	Total skilled ICT workers (%)
FC_TIC	Total number of firms with ICT training programs for employees (%)
G_TIC	ICT training expenses (thousands Euros)

Table 1. Industrial employment variables

LAN	Firms with local area network (%)		
LAN_WL	Firms with wireless local area network (%)		
INTERNET	Firms with Internet connection (%)		
EXTRANET	Firms with extranet connection (%)		
GTIC_R	Ratio ICT regional expenses/ total ICT nation expenses (%)		
E_EMP	Ratio(Regionindustrialemployment)/(Nationindustrialemployment)		
E_IND_9606	Industrial employment variation (1996-2006)		
E_SERV	Services employment variation (1996-2006)		
E_SERV_SI	Information services society employment variation (1996-2006)		
EM2006_R	Ratio industry employment/ total nation employment		
DIF_ETIC	Firms with difficulties on enrollment of skilled, user level, ICT (%)		
VAB_IND_9606	Gross added value industry variation (96-06)		
R_VAB06	Ratio Gross added value region/ Nation gross added value		

To estimate the effects on industrial employment of the ICT diffusion, a model of structural equations was applied whose representation is in graph 2.

Graph 2. Structural equations model



To alleviate the problem of the reduced sample size, 17 regions, and confirm the FIML results, these were checked applying bootstrap and Bayesian methods (results not included here) finding no significant differences.

RESULTS

The industrial employment survey data show that the Madrid region reduced the employment in this sector in almost 14.000 people in the 1996-2006 period. This tendency is similar to the one of Catalonia region, where the industrial employment decreased, according to National Statistical Institute (INE) data, in roughly 17.000 people. However, the rest of regions registered net increases on the number of employees in industry. This way, the tendency experienced in the group for Spain was, on the whole, more positive being created slightly more than 200.000 jobs in the along the period. In absolute terms Madrid and Catalonia are, according to 2006 data, the two regions with more industrial employment. Together both regions added 862.625 jobs in this sector, 32,8 % of the industrial employment in Spain. In addition, both regions generated a strong growth of the employment in the services sector in this period that compensated the fall of the industrial employment. Is there any relationship between this increment and the employment increase in the services sector observed in the last years? To answer this question, the table 2 shows the model coefficients.

In what concerns to the first part of the effects (chart 2.A) -those that influencing the industrial employmentit is necessary to highlight three types of effects: 1) those related with the sector services, 2) the relatives to the ICT, 3) the incidence of the growth of the industrial VAB. In what follows, the main results are analyzed, being indicated, among parenthesis, the standardized values and their p-value.

In what concerns to the first one, the services, the results indicate that there is a negative effect of the growth of the employment in the services of society of the information (variable E_SERV_SI) that is statistically very significant (E_SERV_SI=-0,137; p=0,005). This means that those regions, like as Madrid that registered worse industrial employment evolution also registered growths in the ICT sector. It is also established that there is certain negative incidence (variable E_SERV) of the employment growth in the sector services in the industrial employment (E_SERV=-0,214; p=0,31), nevertheless, less significant (69% confidence level).

 Table 2.
 Model estimated parameters

Explained variable	Indicator	Standardi zed Not	Stand	S.E	C.R.	p- value
A. Industry employment variation effects						
E_IND_9606	E_SERV	-0,214	-0,167	0,165	-1,02	0,31
E_IND_9606	E_SERV_SI	-0,317	-0,233	0,082	-2,84	0,005
E_IND_9606	EXTRANET	-0,284	-1,415	0,889	-1,59	0,111
E_IND_9606	DIF_ETIC	0,194	0,39	0,371	1,05	0,293
E_IND_9606	LAN_WL	-0,414	-1,902	0,628	-3,03	0,002
E_IND_9606	VAB_IND_960 6	0,717	0,78	0,222	3,52	***
B,Industry effects						
EM2006_R	E_IND_9606	0,070	0,029	0,016	1,79	0,073
EM2006_R	R_VAB06	0,760	0,676	0,084	8,00	***
EM2006_R	NEMP	0,273	0	0	3,04	0,002
VAB_IND_96 06	DIF_ETIC	-0,543	-1,003	0,387	-2,59	0,01
R_VAB06	LAN_WL	0,363	0,778	0,46	1,69	0,091
R_VAB06	EXTRANET	0,389	0,904	0,499	1,81	0,07
A. Other effects						
E_SERV	VAB_IND_960 6	0,875	1,218	0,261	4,66	***
E_SERV	DIF_ETIC	0,725	1,863	0,483	3,86	***
EXTRANET	E_SERV	-0,644	-0,101	0,025	-4,12	***
EXTRANET	LAN_WL	0,443	0,408	0,144	2,84	0,005
NEMP	R_VAB06	1,084	6042,1	506,9	11,92	***
NEMP	EXTRANET	-0,301	-3896,6	1178,	-3,31	***
				1		

The second group of variables with incidence on the industry employment growth is the ICT use. Here it is necessary to highlight, in the first place, the negative effect on the of the employment growth of the extranet use (EXTRANET =0,284; p=0,111) and the use of own wireless net (LAN WL=0,414; p=0,002). This negative incidence has its base in the positive relationship that exists between the productivity and the technology. A technological improvement is translated into productivity growth and, as consequence, in a smaller employment need to generate the same production before this advancement. The industrial activity is a typically an intensive technology sector where the margins of the companies depend more and more of the capacity to adapt technological advances to its production chain. This way, the incorporation of the ICT to the industry is reflected in terms of smaller employment need. The difficulty of hiring skilled ICT workers doesn't have significant effects although, with a 70,7%, confidence level has a positive correlation on regions with bigger employment growth. A third relative aspect to the growth of the industrial employment incorporated in the model is the growth of the industrial VAB (VAB_IND_9606). As expected, earnings in the gross added value are reflected in more need of industrial employment (VAB IND 9606=0,717; p < 0,001).

On the other hand, a second group of estimates highlights some of the factors that have affected the recent industry evolution (chart 2.B). Essentially, being the biggest the ICT effect on the added value. The regions where there is more penetration of the ICT, are in fact in those where industry has bigger relevance (LAN_WL=0,363;p=0,091;EXTRANET=0,389;p=0,07). In addition, the difficulties to find skilled ICT workers are shown as a factor that impedes the biggest growth in the added value (DIF_ETIC=-0,543; p=0, 01). These results reveal the necessity on the part of the authorities of promoting the ICT skills on workers and the installation of technological advances in the companies. The conjunction of both factors will improve industry long term the results.

A last group of effects reveals aspects of importance that corroborate the previously described (chart 2.C). Regions with bigger growth of the industrial production have also registered bigger employment growth of the sector services (VAB_IND_9606=0,875; p <0,001). This way, since the growth of the industrial VAB takes place, mainly, based on productivity growths, it is the sector services the one capturing that work force. This fact confirms the results of chart 2A.

It is necessary to highlight, additionally, the positive correlation among the difficulties to find skilled ICT workers in the industry and the employment growth in the services sector (DIF_ETIC = 0,725; p <0,001). This is, as much as is the difficulty to find specialist skilled ICT workers is bigger the growth of the employment on the services sector. This is logical if, also, one keeps in mind the negative relationship, already noted, between the employment growth in the information society segment and the industrial one.

CONCLUSIONS

1. It is necessary to measure the real dimensions of this phenomenon -the creation of net employment in the economic sectors as consequence of the application of the ICT- so that, the employment policies have a reliable bases where to stand on. After several years of analysis, the economic and social effects of Internet continue surprising even the experts.

2. It is needed to better understand the possibilities of the use of the technology and their implications in the regulation.

3. The education policy should be directed toward the use of the digital technologies. For societies obtain the advantages of the ICT requires that the great majority of

the citizens has the necessary knowledge to participate in the digital economy.

4. It would be necessary the regular use of the computers in all the educational levels as well as in management courses.

5. The widespread use, in the formative centers, of the software necessary for the respective profession would confer an advantage to them, and would be a factor for the attraction, to hire its students, of the companies creating employment.

6. Considering the effects affecting the variation of the industrial employment - it is necessary to highlight:

1) Those related with the services sector, where the regions that shown a worse evolution of the industrial employment shown growth in the information society sector services, this being technology intensive, and a slight negative incidence on the employment growth in the sector services in general and in the industrial one.

2) Those related to the ICT. Where two variables have a negative effect on the employment growth: the extranet use and the use of their own wireless net. This negative incidence has its base in the positive relationship that exists between productivity and technology. This way, the incorporation of the ICT to the industry is being reflected in terms of smaller employment need.

7. A second group of estimates reveals some of the factors that have influenced the industry recent evolution. The most prominent outcome is the effect of the ICT in the added value. The regions with more ICT diffusion are those with bigger industry relevance on the Spanish economy. In addition, a difficulty to find skilled ICT workers is a factor that impedes a biggest added value growth. These results reveal the necessity on the part of the competent authorities to expand a qualified work force and the installation of technological advances in the companies. The conjunction of both factors will improve the industry long-term results.

8. A last group of effects reveals that regions with bigger growth of the industrial production have also bigger growth on the sector services employment.

9. An important aspect, not approached in this work, it is determining how many employments have been kept due to the ICT effect on competitiveness.

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MORTALITY RATES OF SPANISH DEPENDENTS: A JOINT CORRECTION APPROACH

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KEYWORDS

dependents, long term care insurance, extramortality, correction of mortality rates.

ABSTRACT

The quantification of mortality, especially the one corresponding to the dependents insured, is nowadays a core problem when pricing long term insurance. The usual fit in Spain shows a big gap, even more important when adjusting older ages. What we show and present in the following pages is a joint correction of the extramortality rates departing from the well-known Rickayzen and Walsh reciprocal function of one plus an exponential. When comparing it wit the usual additive and multiplicative corrections, the joint one yields better results, fitting better to the real Spanih sutuation and thus should be choosen and applied by the insurance sector when working on the subject.

INTRODUCTION

A key element in the pricing of long term care insurance is the quantification of mortality, especially the one corresponding to the dependents insured.

In the actuarial literature on mortality of the dependents insured, there is an unanimous opinion in regard to the mortality rates of dependents are different and higher than those of the overall mortality expressed in general mortality tables used by insurers for the valuation of normal hazards, and of course, appreciably higher than the mortality of insured autonomous. The following expression is therefore assumed:

$$q_x^d > q_x > q_x^a \tag{1}$$

A different question is, and resolved through different procedures too, the treatment given to the mortality rates when it comes to measure and to express in a mathematical way the present asseveration. Then, there is no single approach but, in contrast, different corrections can be found of the overall mortality for heads in situation of dependence. The first step in the delivery of adjusted mortality rates consists in having a mortality table of heads in a state of dependence, with gross values, whose definition corresponds to the contractually used in the policy as the one generating benefits in a long term care situation, and that employs equivalent criteria for obtaining the ranking of the long term care situation to those used in the derivation of the incidence rates. The starting raw data come from French survey HID 98-01.

Differences in the mortality of dependents, according to its level, induce not just higher and different overmortality values but also the functional expressions in which these values are modelled, so it's usually associated additive adjustments to the great dependencies and multiplicative to the less severe ones, as can be seen in (Gatenby 1991).

Once raw mortality of dependents data are derived, different formulas are proposed for correcting these mortality rates; the chosen procedure will minimize the squared deviations function.

Base table for correction

The mortality of dependents is usually derived from overall mortality statistics or mortality of healthy heads. In this case annuity tables are chosen because in this business insurer must also face the survival risk, as (Pitacco 2002) evidences. In the present paper we will fit French statistics, HID 98-01, corrected for Spanish population, using as base statistics the PERMF-00P tables.

Adjustment of mortality rates

There are different ways to adjust the mortality rate of the insured in a long-term care situation, all of them using as a starting point the following expression due to (Ainslie 2000).

$$q_x^d = q_{x+\delta} \times \beta(x) + \alpha(x) \tag{2}$$

where

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 $\beta(x)$ Factor of the general mortality rate, that can be depending on the age;

 $\alpha(x)$ Additive surcharge on the overall

mortality, which may depend in turn on the age δ Whole number of years to add to the

overall mortality rates.

There are then different approaches, all deriving from the previous general form, depending on the different functional expressions that the general formula finally takes. The choice of a specific fit will finally turn on the level of dependence which in turn is closely related to the kind of pathologies generating the state of long-term care.

The usual correction by adding years to the standard mortality rate hazards is frequently replaced using multiplicative or additive factors, or a mixture of them, even if they don't yield the same values. In the present paper the fitting of the extramortality will not follow that way.

The best approach to the raw mortality data of the great dependents corrected for the Spanish population will come from the comparison of them to the chosen standard mortality tables, the PERMF-00P ones.

THE ADDITIVE CORRECTION

In case that, in the general calculation formula, equals to one, the correction over the overall mortality rates will follow the additive correction. That family shows different fitting possibilities, either through a fixed constant either through other sort of corrections directly depending on the age. We will follow the additive correction proposed by Rickayzen and Walsh known as "reciprocal of one plus an exponential".

Fixed correction

In addition to its simplicity, this type of adjustment has the property that, as indicated in Ainslie, its weight decreases, in relative terms, with regard to the overall mortality, which is always increasing in the range of ages of elderly.

The materialization of the mortality of dependents under this assumption would remain as

$$q_x^d = q_x + \alpha \tag{3}$$

This correction has been widely used in actuarial literature because it better fits the mortality of great dependents than other sort of approaches, and its implementation is quite easy. See, for instance, MacDonald and Pritchard ; they propose an additive correction for Alzheimer's institutionalized sufferers of 0.17291. Gatenby considers a value of 0.1 for the extramortality of dependents.

The derivation of the fitting parameters is done through ordinary least squares (OLS) (López shows a comprehensive explanation of the use of OLS for deriving the parameters) and yields the following results :



Figure 1: Raw differentials in the mortality rates of dependents and its fit. Additive adjustment from a fixed correction

The additive fit from a fixed correction overestimates the extramortality in younger ages and underestimates those from elderly. This same effect can be seen in overall mortality values already adjusted for dependents, showing that this fitting procedure is not the most appropriate one.



Figure 2: Mortality rates for great dependents. Raw vs. fitted data Additive adjustment from a fixed correction

Age-dependent correction

This additive fitting procedure over the overall mortality rates has the advantage of considering age as an independent variable in a functional way.

The approach to the overmortality proposed by Rickayzen and Walsh in the modelling of the UK data fall into this type of corrections. Because of the lack of British data, they use raw data from the USA, derived from the report of the Society of American Actuaries (SOA), which considers data of the log-term care surveys between 1982 and 1984. The statistics of transition states were obtained from people who were receiving benefits from the Medicare public system. As a result it was observed that:

•Mortality rates increase with the disability level.

•The mortality ratio among those failing more than 3 activities of daily living (ADLs) and those not failing any decreases with age.

•The differences in mortality among those who fail over 3 ADLs and those not failing any has, roughly speaking, an additive behaviour in mortality with a value of 0.15.

With these starting premises Rickayzen and Walsh propose an additive correction from a reciprocal function of one plus an exponential of the following type:

$$q_x^d = q_x + \frac{\delta}{1 + \lambda^{x_i - x}} \qquad (4)$$

where

 δ Maximum value (of asymptotically convergence) to incorporate depending on the age.

 λ Slope factor

 x_i Inflection age where the curve changes its shape, from convexity to concavity.

This sort of additive modification of mortality is based on the following considerations, that characterize the proposed function and that is used in both Rickayzen and Walsh as in Leung :

•There is a weak relationship between the mortality of healthy heads and the one of those who are dependents; •The overmortality is significantly lower in younger ages;

•For less severe dependencies no overmortality is applied.

In our paper the derivation of the , and values come from an OLS procedure with regard to the Spanish gross-up estimated great dependency data, according to the following expression :



Figure 3: Raw differentials in the mortality rates of dependents and its fit Additive adjustment. Rickayzen and Walsh proposed correction

This additive age-dependent adjustment fits much better the overmortality than the fixed correction additive one. The already mortality-adjusted overall values for dependents under this procedure are shown in the following figure.



Figure 4: Mortality rates for great dependents. Raw vs. fitted dataAdditive adjustment. Rickayzen and Walsh proposed correction

THE MULTIPLICATIVE CORRECTION

Taking the general expression for a null $\alpha(x)$ we will find a multiplicative correction of the overall mortality rates according to the following expression:

$$q_x^d = q_x \times \beta(x) \tag{5}$$

Fixed correction

As the prior case of additive fixed correction, this easy to implement procedure and its very intuitive interpretation justifies its widely use, especially for those less severe dependence levels. The disadvantage this method presents comes from its poor adjustment for great dependencies because these statistically weakly depend on overall mortality rates. In the figure below we can appreciate this assertion, after fitting through OLS the differential of mortality among tables PERMF-00P and mortality for great dependents, considering the Spanish modified HID 98-01.



Figure 5: Raw differentials in the mortality rates of dependents and its fit Multiplicative adjustment with fixed correction

The overall values of mortality for dependents under this procedure, shown in the following figure, reflect the bad mortality fit for them:



Figure 6: Mortality rates for great dependents. Raw vs. fitted data Multiplicative adjustment with fixed correction

Age-dependent correction

In order to improve the goodness of the previous fit, from a multiplicative modification of mortality rates, and taking into account, as observed in SOA, that the ratio of the mortality of dependents with regard to the overall mortality decreases with age, some authors propose a correction of the multiplicative fit. Boladeras proposes a linear overmortality age-decreasing correction, according to the next expression :

$$q_x^d = q_x \times \max\left[\left(\omega - x \cdot \varphi\right); 1\right] \quad (6)$$

where

 ω Maximum multiplicative correction to take into consideration on the standard mortality rates to reflect the mortality of dependents.

 φ Reduction on the mortality rates of dependents applied to each age

The figure below reflects the OLS fit of the differential of mortality among PERMF-00P tables and mortality for great dependents, considering the Spanish modified HID 98-01 using the multiplicative age-dependent correction.



Figure 7: Raw differentials in the mortality rates of dependents and its fit Multiplicative adjustment with age-dependent correction

Our results for the present fitting considerably differ from those from Boladeras, with notably different values for men and women. In case of men, equals to 18.90 and takes a value of 0.1731, as the values for women are 20.59 and 0.1954 respectively.

The overall values of mortality for dependents under this procedure, shown in the following figure, reflect a better fit in the mortality of dependents than in the case of the fixed multiplicative correction:



Figure 8: Mortality rates for great dependents. Raw vs. fitted data Multiplicative adjustment with age-dependent correction

The achieved results in the latest modelled ages, with declining mortality rates, do not recommend the use of this fitting procedure.

JOINT CORRECTIONS

Corrections with additive and multiplicative amendments are employed together to fit the extramortality; they try to by-pass the deficiencies of the prior studied procedures, incorporating on one hand a mortality not linked to the overall mortality rates, and on the other a mortality depending on the behavior of the overall mortality.

Linear correction

The linear correction, which considers the overall mortality as the independent variable, is the more widespread case. So we have

The OLS fit of the mortality differential among PERMF-00P tables and great dependents mortality considering the Spanish modified HID 98-01, using the joint linear correction, yields the following results:



Figure 9: Raw differentials in the mortality rates of dependents and its fit Joint linear adjustment

As in the case of fixed multiplicative correction, this approach overestimates the additional mortality of dependents in ages under 60 and underestimates the one for those over 70 years.

The aggregated mortality values for dependents according to this procedure, as shown in the following figure, evidence the lack of the fit in the mortality of dependents:



Figure 10: Mortality rates for great dependents. Raw vs. fitted dataJoint linear adjustment

Modified Rickayzen and Walsh correction

The fitting function proposed in Rickayzen and Walsh fits overmortality according to an additive expression of a reciprocal function of one plus an exponential. This fit raises the convergence of overmortality to a maximum value of . This method yields satisfying results if the modelled differentials do not decline after a certain age. With the GK-95 y GR-95 mortality tables there's no declining so the fit is excellent. However the ovemortality differentials respect to the PERMF-00P table decline for both genders after the age of 96. To reflect this effect, we now propose a departure from the Rickayzen and Walsh original formula from a joint correction of the overall mortality to adjust the mortality of dependents. In the present joint correction we consider an additive correction according to the Rickayzen and Walsh expression and a multiplicative correction over the overall mortality rates reflecting the declining of the absolute mortality differentials in the

highest ages of the table. Therefore, we get the mortality of dependents from the following formula:

$$q_x^d = q_x \times \beta + \frac{\delta}{1 + \lambda^{x_i - x}} \tag{7}$$

The figure below reflects the OLS fitting of the mortality differential among PERMF-00P tables and the mortality for great dependents considering the Spanish modified HID 98-01 using this joint correction.





As the figure shows, the fit reflects the decreasing differential among the mortality of healthy individuals and people in state of great dependence after 95 years. The results in the overall mortality with this joint correction, by age and gender, are reflected in the figure below:



Figure 12: Mortality rates for great dependents. Raw vs. fitted data Joint adjustment with additive age-dependent correction

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Modelling, Simulation and Control of Technological Processes

NONLINEAR MODEL FOR RECIPROCATING EQUIPMENT PISTON ROD ELASTIC PLASTIC DEFORMATION

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KEYWORDS

Reciprocating Equipment, Nonlinear Deformation, Piston Rod.

ABSTRACT

Reliability assessment of reciprocating equipment piston rod leads to nonlinear elastic-plastic deformation analysis of rod with initial imperfection under axial dynamic load. In this paper a new and effective model and analytical simulation method are presented to evaluate dynamic deformation and elastic-plastic stress of reciprocating machine piston rod. This new method has capability to account for geometric nonlinearity, elastic-plastic deformation and dynamic effects. Proposed method can be used for evaluation of piston rod performance for various reciprocating machines under various operation situations. Rod load curves and maximum allowable rod load are calculated with presented method for a reciprocating compressor. Useful recommendations and guidelines for rod load, rod load reversal and rod drop monitoring are also addressed.

INTRODUCTION

Reciprocating machines (reciprocating compressors, reciprocating pumps, gas and diesel engines, reciprocating expanders, etc) are most efficient available machines (Bloch 2006a; Bloch and Hoefner 1996; Brown 2005). These machines are vital components in industrial plants. There are flexible to handle wide capacity and condition swings. In many cases the reliability of plant is dictated by the reliability of the reciprocating machines. Important topics related to these machines are rod load and piston rod reliability (Wilson 2007). Reliability assessment of reciprocating machine piston rod leads to nonlinear deformation analysis of rod with initial imperfection under axial dynamic load. It presents a real challenge due to complex nonlinear deformation, elastic-plastic behavior and dynamic effects. Previous proposed Finite Element Methods (F.E.M.) are restricted in various limits and uncertainties and relatively accurate results need countless meshes, continual re-meshing and other special considerations. The reciprocating machine rod is subjected to a combination of fluid (gas in compressors and engines and liquid in pumps) and inertia (of reciprocating and rotating components) loads. Rod load can be influenced by changes in operating pressures, capacity changes (Hickman 2007; Leonard 1996; Schultheis et al. 2007), unloading, valve leaks and other causes. Rod loading must be kept within the limit set because overloading can cause excess run out of the rod resulting in premature packing wear, leakage, reduced efficiency, increased maintenance expense and potential of catastrophic failure including risk of personnel injury (Fagundes et al. 2004; Hickman 2007; Leonard 1996; Schultheis et al. 2007). Also with the pollution laws becoming more stringent, leakage control takes on a much greater significant.

This paper presents model, formulation and simulation routine for predicting piston rod deformation and rod load limit. This formulation and routine can be used to generate machine loading tables and rod run-out values that permit operators to load machines confidentially at rated capacity for best efficiency and maximum throughput. Without these data, low confidence placement may lead to low load factor and low capacity or serious effects of overloading.

MODEL FOR PISTON ROD

Experience with high pressure reciprocating machines revealed that piston rod problems are important sources of machine failure and machine unexpected shut down for repair. These failures consisted of severe scuffing and wear between sealing element (piston and packing rings) and the counter surface (liner and piston rods) causing erratic seal life, sometimes only a few hours duration, together with badly damage cylinder liners and piston rods. The rod load varies from compression to tension and vice-versa along the piston stroke. Load carrying limit referred as rod load or frame load is maximum continuous operating force that machine can safely and reliability withstand. It is load that can be borne by the crankshaft, connecting rod, frame, piston rod, bolting and bearing. Knowledge of rod load has great effect on reciprocating machine safety and reliability. There were many reports about insufficient accuracy in the machine manufacturer's rod load data. Discrepancies more than 20% were reported between machine manufacturer load curves and reciprocating machine site performance results (Bishop 1985). For old machines reported differences and discrepancies are considerably higher. For safe and reliable operation, operators should be furnished with accurate and reliable rod load data because operating conditions and

pressures can be varied due to many reasons. Operator shall be able to keep machine running confidentially and safely using proper data and load tables and curves. It is necessary to develop a more precise method for prediction of reciprocating machine rod loads. The rod load depends on the cylinder fluid pressure and reciprocating machine component inertia forces. One of the most important issues in this regard is piston rod deformation and piston rod load bearing capacity which will be addressed in this paper. In many cases rod stress or deformation can be the limiting factor or the "weakest link in the chain".

Axial position of the piston depends upon crank angular position and connecting rod-crank ratio. The piston velocity is zero at beginning of the stroke and decrease zero at the end of stroke. Piston acceleration is maximum at each end of the stroke where piston changes direction. Acceleration is zero near mid-stroke where the velocity is maximum. Forces acting on reciprocating machine moving parts are: 1- cylinder fluid pressure forces 2- inertia and dynamic forces of reciprocating parts 3- centrifugal forces of rotating parts. The cylinder fluid pressure forces are main loads. Inertia, dynamic and centrifugal forces are usually considerable for big machines (with heavy moving masses) or high speed machines (Gajjar 1996). The total load of cylinder fluid is found by a simple multiplication of the pressure times the piston area. If the piston is double-acting, the sum of loads on head end and crank end of piston must be taken into account. The inertia rod load is proportional to the square of machine speed. Inertia loads become important for large and heavy pistons, high speeds or little pressure differences. In most cases combined loads (fluid plus inertia) are lower than the fluid loads. This may not be true for low pressure ratio (high volumetric efficiency) applications. As an approximate rule, if the discharge Volumetric Efficiency (VE) is less than 50% (which is very common), the fluid load will reach a maximum after the 90 degrees, so it is opposite in sign to the inertia load. In this paper main concern is rod deformation of process reciprocating machines which have normally slow speed and high pressure differences. Inertia loads are small compare with fluid loads for these machines. However both cylinder fluid load and inertia load are considered in presented model and simulation. It is necessary to note that in-cylinder pressures are different with nominal pressures due to several effects such as valve and cylinder passage losses (typically 2-10% difference), pulsation control devices (around 1% difference), cylinder valves (typically < 7%difference) and valve dynamics (inertia, sticktion, flutter, etc). These effects shall be addressed in accurate rod load calculations.

Only axial loading is considered and only transverse inertial are taken into account. Figure (1) presents model for piston rod elastic-plastic nonlinear deformation.



Figure 1: Model for Piston Rod Elastic-Plastic Nonlinear Deformation.

The elastic-plastic deformation in form of elastic-plastic hinge takes into account the coupling effects between bending and compression. Large numbers of elements in the elastic-plastic hinge (more than 30) are considered to obtain accurate results. Figure (2) shows model for elastic-plastic hinge assumed in middle of piston rod. This model can simulate the progression of thin plastic zones in both sides of rod cross section. This elasticplastic nonlinear deformation can model small values of run out resulted from overloading. Piston rod is modelled by an initially imperfect rod with initial length $(2L_o)$ with reference to Figure (1). As noted there is an assumed elastic-plastic hinge in the middle of rod. Initial imperfection is shown by (y_o) . Mass (m_R) is assumed concentrated mass at elastic-plastic hinge in the middle of rod. Parameter (α) and (a) are deflection angle of half of rod and initial half height of middle of the elastic-plastic hinge.



Figure 2: Model for Elastic-Plastic Hinge in Middle of Piston Rod.

FORMULATION

Using "Principle of Virtual Work" (Grzebieta and Murray 1983; Jones and Dos Reis 1980), rod equations of motion can be expressed as Equations (1) and (2). In this equations parameters "F", "y", "M" and "N" are load

transmitted by the rod, transverse deflection of rod due loading, bending moment in the elastic-plastic hinge and force in the elastic-plastic hinge respectively. As noted parameter (α) is deflection angle of half of rod and mass (m_R) is assumed concentrated mass at elastic-plastic hinge in the middle of rod.

$$2F(t)\cos(\alpha(t)) + m_R \frac{d^2 y}{dt^2}\sin(\alpha(t)) + 2N(t) = 0$$
(1)

$$2M(t) - 2F(t)L_o\sin(\alpha(t)) + m_R \frac{d^2y}{dt^2}L_o\cos(\alpha(t)) = 0$$
(2)

Functions "M" and "N" are time dependant moment and force in the elastic-plastic hinge and expressed as Equipments (3) and (4) respectively.

$$N = \cos(\alpha) \sum_{i=1}^{2N} \sigma_i \Delta A_i$$
(3)

$$M = \sum_{i=1}^{2N} \sigma_i \ z_i \,\Delta A_i \tag{4}$$

Parameter " A_i ", " z_i " and " $_i$ " are area of i-th slice of elastic-plastic hinge, abscissa of the middle of i-th slice of elastic-plastic hinge and stress in the i-th slice of elastic-plastic hinge. With respect to presented model, Equations (5) to (7) can be written.

$$a_i(1+\varepsilon_i) = (R+z_i)\sin(\alpha)$$
 (5)

$$L_o \sin(\alpha) = y + y_o \tag{6}$$

$$\boldsymbol{\sigma}_i = f(\boldsymbol{\varepsilon}_i) \tag{7}$$

Parameters " a_i ", " $_i$ " and "R" are half height of middle of the i-th slice of elastic-plastic hinge, strain in the i-th slice of elastic-plastic hinge and elastic - plastic hinge curvature radius. Function "f" in Equation (7) is rod material constitutive strain-stress relation. In the initial state, Equation (8) is valid. As noted " y_o " is initial imperfection of rod and parameter " α_o " is initial deflection angle of half of rod.

$$\sin(\alpha_o) = \frac{y_o}{L_o}$$
(8)

With respect to Equations (1) to (7), rod dynamic deformation, details of stresses and possible permanent deflection can be calculated with knowledge of the force-time relation "F=F(t)" which comes from cylinder fluid and inertial forces of reciprocating machine. End results of these calculations can be maximum allowable rod load for machine using recursive procedure. Material strain rate sensitivity is also considered in formulation (In Equation (7)). To model the strain rate effects, empirical "Cowper-Symond" equation is used.

SIMULATION RESULTS

Figure (3) shows rod load curves (combined gas and inertia load) of heavy duty special purpose reciprocating compressor in refinery service. This rod load and

allowable rod load are calculated based on presented method.



Figure 3: Rod Load Curves for Various Operating Conditions of Reciprocating Compressor.

To calculate allowable rod load, operating run-out is limited to 150 micrometer (6 mils) peak to peak. As indicated, acceptable rod load peak in design condition shall be less than 80% of allowable rod load. However in operating conditions, rod load can be slightly increased to improve machine performance. For this purpose accurate model (such as present model) shall be used and all safety and reliability steps and regulations shall be followed and assured. As shown in Figure (3), variation in suction pressure (in this case low suction, around 7% suction pressure reduction) causes higher rod load. It reminds that all possible process variations especially suction pressure (lower or higher than normal operation) shall be respected in rod load calculation. Working in relief condition (discharge pressure equal by relief valve set pressure) has same effect and can cause higher rod load. Figure (3) shows also that unloading steps can change rod load behaviour and curves. For this compressor, 3/4 flow and 1/2 flow are obtained by clearance pocket and valve unloder respectively. As shown in Figure (3), clearance pocket (3/4 flow) results in slightly lower rod load with same pattern as rod load curve full flow. However valve unloder (unloading one side of double acting cylinder as 1/2 flow) results in completely different rod load behaviour. Actually case of 1/2 flow (valve unloder) shows rod load generated by one side of machine cylinders.

Based on operation experiences and extensive simulations, reciprocating machine capacity can be increased from less than 90% to more than 96% of rated capacity (rated flow) using presented analysis method. For the around 20 MW reciprocating machine station, it yields to more than 300,000 USD annual benefit and fuel saving in addition of maintenance savings. Presented method can also avoid overloading and unnecessary shut down of machines. For a typical heavy duty reciprocating machine in refinery service (for

example in the middle size make up hydrogen reciprocating compressors) each day of shut down means more than 200,000 USD loss of profit.

ROD LOAD REVERSAL RECOMMEDATION

To assure adequate lubrication of the crosshead pin, the load vector should change director during the piston stroke. The combined dynamic piston rod load changes direction from compression to tension. This change in direction allows clearance between the cross head bushing and the cross head pin in the area of the point of lubrication. Similarly, in single acting crank end loading, there is a change in direction of loading along the cylinder axis. The lack of change of direction of the dynamic piston rod load effects on cross head bushing lubrication and heat is generated between the cross head bushing and cross head pin. The heat causes the seizing of the pin with the crosshead bushing. It can result in catastrophic failure.

The lack of direction change is also referred to as "Lack of Reversal". It is necessary to check this issue for all possible operating cases including suction pressure variations, unloading steps, etc. Each reciprocating machine model has own minimum requirement for this reversal. Duration and peak magnitude load of rod reversal shall not less than 15° of crank angle and 3% of the actual combined load in the opposite direction respectively. These minimum requirements shall be checked for all possible operating cases (especially low suction and part load steps) and also proper safety margins shall be respected.

PRACTICAL RECOMMEDATIONS ON PISTON ROD MAINTENANCE AND MONITORING

Emphasis on load monitoring has reduced the instances of overloading while simultaneously raised the average load. In reciprocating machines proximity probes are typically located under the piston rods and are used to measure the rod position (piston rod drop being measured continuously by a proximity sensor). It is to determine wear of the piston and rider bands (Griffith and Flanagan 2001; Leonard 1996; Schultheis et al. 2007).

In the event of a malfunction such as overloading, permanent plastic deformation of rod, a cracked piston rod attachment, a broken crosshead shoe, or even a liquid carryover to a cylinder, the operating rod run-out will increase significantly. Alarm will show excessive run-out. By this monitoring method, malfunction can be found in early stage before major damage. Cold runouts are usually held to about 50 micrometer (2 mils) peak to peak and operating run-outs under normal conditions are typically in the order of 50 to 150 micrometer (2 to 6 mils) peak to peak. Although the theory is simple, getting and interpretation actual online monitoring present challenges. Shut down is not recommended for rod drop monitoring to avoid unnecessary shut down of machine for example in transient cases or monitoring errors. Alarm set point shall also be selected very carefully with respect to all operating conditions, machine current situations, detailed analysis as presented in this paper and experience.

Surveys identified that piston rod and packing life on high pressure reciprocating applications could be improved two and three times by adding the proper tungsten carbide piston rod coating. It is strongly recommended even for small reciprocating machines.

Reciprocating machine can be tested several times annually using electronic analyzer equipment. This practice is cost effective and can reduce maintenance expense through early detection of worn or damage parts. It also verifies cylinder pressures for actual rod load calculation. Pressure velocity analysis is a technique that has proven to be very effective in assessing the condition of reciprocating machinery. Dynamic pressure transducers are used to measure the pressure inside the cylinder over the course of the stroke. This allows the analyst to evaluate the condition of the rod, packing rings, valves, etc, while at the same time measuring the dynamic piston fluid forces for rod load calculation.

The electronic analyzer simulates the indicated mean effective pressure and applies appropriate multipliers for speed and cylinder swept volume to model the rod load and power. One type of analyzer simulates piston velocity, and thus volume, with voltage generators. Another type of analyzer uses a digital computing device to calculate a table of volume increments as a function of crank rotation. It is beyond the scope of this paper to provide an assessment of electronic analyzer detail and accuracy. Simply stated the analyzer monitors the pressure and relates it to volume by tracking the crankshaft motion. This monitoring technique is strongly recommended.

CONCLUSION

In many cases the reliability of plant is dictated by the reliability of the reciprocating machines. Important topics related to these machines are rod load and piston rod reliability. Safety, reliability and service life of reciprocating machines depend to a large extent on the operating of the piston rod mechanisms and related packings. In this paper an effective analytical model and simulation method are presented to evaluate reciprocating machine rod deformation. Presented method is able to account for geometric nonlinearity, elastic-platic deformation, dynamic effects and different loading profile of various reciprocating machines. Analytical simulation results are discussed. Useful recommendations and guidelines for rod load, load reversal and rod drop monitoring are also presented.

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USING OF SELF-TUNING CONTROLLERS SIMULINK LIBRARY FOR REAL-TIME CONTROL OF NONLINEAR SERVO SYSTEM

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KEYWORDS

Self-tuning control, ARX model, recursive least squares, LQ control, polynomial approach, MATLAB–Simulink, servo motor, real-time verification

ABSTRACT

The combination of the automatic control theory courses, simulation verification and practical implementation of the designed controller algorithms in real-time conditions is very important for training of the control engineers. This contribution present structure and usage of Self-tuning Controllers Simulink Library (STCSL) for real time control. The STCSL was created for design, simulation verification and especially realtime implementation of single input - single output (SISO) digital self-tuning controllers. The proposed adaptive controllers, which are included in the library, can be divided into three groups (PID controllers, controllers based on the polynomial approach and the controllers derived on the other approaches (minimum variance etc.). This Library is very successfully used in Adaptive Control Course in education practice for design and verification of self-tuning control systems in simulation and real-time conditions. It is suitable also for design and verification of industrial digital controllers. The highly nonlinear laboratory model, the DR300 Speed Control with Variable Load, has been chosen as example for real-time control. The STCSL is available free of charge at the Tomas Bata University internet site - http://www.utb.cz/stctool/.

INTRODUCTION

One approach to adaptive control is based on recursive estimation of unknown system characteristics, gradually specifying them, and then monitoring possible changes. Using this knowledge, appropriate methods can be employed to design the optimal controller. This kind of controller, which identifies unknown processes and then synthesizes control (adaptive control with recursive identification), is referred to in the literature as a *selftuning controller* (STC). Self-tuning controllers use the combination of the recursive process identification based on a selected model process and a controller synthesis based on knowledge of parameter estimates of controlled process. In some STCs, the identification process does not serve to determine the estimates of the process model parameters $\hat{\Theta}(k)$; rather, appropriate reparametrisation of the control loop can be used recursively to estimate the controller parameters directly. Therefore, it is necessary to find the relationship between the process input and output and define it straight from the controller parameters without recalculating them using the estimates of the process model parameters. These controllers are referred to as being *implicit*, whereas controllers using a synthesis from estimates of the process model parameters are called *explicit* (with direct identification).

Presently, most of the explicit STCs are based on the Certainty Equivalence (CE) Principle. The basic principle of CE is that the model uncertainty is not considered. The parameter estimates of the process model, which are obtained by recursive identification, are used for the controller design. It is assumed that values of these estimates correspond to their actual values.

The aim of this contribution is not only to inform potential users about Self-tuning Controllers Simulink Library - STCSL (see Bobál and Chalupa, 2002) and to provide help for usage of the library in the simulation verification (see Bobál et al. 2008) but also to demonstrate the practical approach to a design of a control of the laboratory model in real-time conditions.

RECURSIVE IDENTIFICATION

The regression (ARX) model of the following form

$$y(k) = \boldsymbol{\Theta}^{T}(k)\boldsymbol{\Phi}(k-1) + n(k)$$
(1)

is used in the identification part of the designed controller algorithms, where

$$\boldsymbol{\Theta}^{T}(k) = \left[a_{1}, a_{2}, ..., a_{na}, b_{1}, b_{2}, ..., b_{nb}\right]$$
(2)

is the vector of the parameters and

$$\boldsymbol{\Phi}^{T}(k-1) = \begin{bmatrix} -y(k-1), -y(k-2), \dots, -y(k-na), \\ u(k-1), u(k-2), \dots, u(k-nb) \end{bmatrix}$$
(3)

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) is the regression vector (y(k)) is the process output variable, u(k) is the controller output variable). The non-measurable random component n(k) is assumed to have zero mean value E[n(k)] = 0 and constant covariance (dispersion) $R = E[n^2(k)]$.

The recursive least squares method for calculating of parameter estimates $\hat{\Theta}(k)$ is utilized. Using the pure least squares method, the influence of all pairs of identified system inputs and outputs to the parameters estimates is the same. This property can be inconvenient for example when identifying a system with time-varying parameters. In this case, it is better to use least squares method with exponential forgetting where the influence of latter data to the calculation of the parameter estimates is greater then the influence of older data.

The exponential forgetting method can be further improved by adaptive directional forgetting (Kulhavý, 1987) which changes forgetting coefficient with respect to changes of input and output signal.

CONTROLLER ALGORITHMS

The proposed self-tuning controllers which are included in the library are divided into three groups:

- classical digital PI and PID controllers whose tuning is based on Ziegler-Nichols method, pole assignment method and its modifications,
- controllers based on polynomial approach (deadbeat strong and weak version, pole assignment, controllers based on minimization of quadratic criterion),
- controllers based on other approaches (minimum variance controllers, Dahlin's controller, Bányász-Keviczky's controller etc.).

SELF-TUNING CONTROLLERS SIMULINK LIBRARY

The Simulink is nowadays a word-wide standard in simulation, testing, and verification of behaviour of various dynamic systems. Simulink is a part of MATLAB system and supports linear or nonlinear systems modelled in continuous time, sampled time or a hybrid of the two. Systems can also be multirate, i.e. have different parts that are sampled or updated at different rates.

Based on monograph Bobál, et al. (2005) a library of self-tuning controllers in MATLAB/Simulink environment was created. The purpose was to create a framework suitable for creating and testing of self-tuning controllers. The library is available free of charge at internet site of Tomas Bata University in Zlín – www.utb.cz/stctool/ (see Bobál and Chalupa, 2002). The library was created using MATLAB version 6.5 (Release 13) and is compatible with all newer

MATLAB versions. Controllers are implemented in the library as standalone Simulink blocks, which allows an easy incorporation into existing simulation schemes and an easy creation of new simulation circuits. Only standard techniques of Simulink environment were used when creating the controller blocks and thus just basic knowledge of this environment is required to start working with the library. Controllers can be implemented into simulation schemes just by the copy or drag & drop operation and their parameters are set using dialog windows. Another advantage of the used approach is a relatively easy implementation of userdefined controllers by modifying some suitable controller from the library.

Nowadays the library contains over 30 simple single input single output discrete self-tuning controllers, which use discrete ARX models of second and third order for the on-line system identification.

DESCRIPTION OF LABORATORY MODEL AMIRA DR300

Some of self-tuning algorithms were tested using a realtime laboratory model DR300 (Speed Control with Variable Load) by the Amira Company, Duisburg, Germany (see Fig. 1).



Figure 1: Laboratory Model Amira DR300

A simplified scheme of the DR300 system is shown in Fig. 2.



Figure: 2: Simplified Scheme of Amira DR300 Laboratory servo System (*u*:Motor Control Voltage; M: DC Motor; S: Motor Shaft Rotation Sensor)

The rotation speed of the motor M is driven by voltage u. The motor shaft rotations per minute (rpm) are measured by sensor S. The aim of the control process is to control the rotation speed of the shaft by the control voltage u.



Figure 3: Static Characteristics of DR300 Servomotor

From the control point of view, the Amira DR300 is a nonlinear system. Some characteristics of the nonlinearity can be observed from the static characteristics shown in Fig. 3.

EXPERIMENTAL RESULTS

Many different setting of the self-tuning controller from the STCSL (Bobál, Chalupa 2002) were applied to the Amira DR300 system and some results are presented in this chapter.

Interconnection of a MATLAB/Simulink and the Amira DR300 system was realized using Real-Time Toolbox (RTT) and the MF614 data acquisition card (both by Humusoft). The Real-Time Toolbox allows direct connection of the Simulink and a real-time controlled system without any restrictions concerning the programming language that is used for user-defined Simulink functions. Contrary to Real-Time Workshop, the RTT can use whole set of MATLAB functions and toolboxes. Main drawback of usage RTT consists in the fact that the toolbox cannot produce source code for stand-alone controlled systems.

The LQ based controller pp2lq was used as a base for comparison with other controllers and setting. Computation of the control sequence of the pp2lqcontroller is based on minimization of a quadratic criterion in the following form (Bobál et al. 2005). The coefficients of the characteristic polynomial $D(z^{-1})$ of the closed loop are computed to minimize the LQ criterion (4):

$$J = \sum_{k=0}^{\infty} \left\{ \left[w(k) - y(k) \right]^2 + \lambda \left[u(k) \right]^2 \right\}$$
$$D(z^{-1}) = 1 + d_1 z^{-1} + d_2 z^{-2} \qquad (4)$$
$$d_1 = \frac{m_1}{\delta + m_2}; \quad d_2 = \frac{m_2}{\delta}$$

The parameters m_1 , m_2 and δ are computed as follows:

$$\delta = \frac{\gamma + \sqrt{\lambda^2 - 4m_2^2}}{2}; \quad \gamma = \frac{m_0}{2} - m_2 + \sqrt{\left(\frac{m_0}{2} + m_2\right)^2 - m_1^2}$$
$$m_0 = \lambda \left(1 + a_1^2 + a_2^2\right) + b_1^2 + b_2^2; \quad m_1 = \lambda (a_1 + a_1a_2) + b_1b_2 \quad (5)$$
$$m_2 = \lambda a_2$$

where λ is a coefficient representing weight of control signal increments in the LQ criterion.

The LQ controller of 2DOF (two degrees of freedom) structure was applied in the form

$$u(k) = r_0 w(k) - q_0 y(k) - q_1 y(k-1) - q_2 y(k-2) + + (1-p_1) u(k-1) + p_1 u(k-2)$$
(6)

The expressions for computation of individual controller parameters are introduced in Bobál, et al. (2005).

The sample time $T_0=0.05$ s, penalization of control sequence $\lambda=5$ (denoted as "Penalization of controller output – fi" in the STCSL) and on-line identification with the adaptive directional forgetting was used as a nominal case. Control courses obtained by these settings are presented in Fig. 4.



Figure 4: Control Courses of the Nominal Settings of pp2lq Controller ($T_0=0.05$, adf, $\lambda=5$)

While courses presented in this figure are in physical units, the values of the controller input and output were normalized. The normalized controller inputs in the range $\langle -1, 1 \rangle$ represented rotation speed of the shaft in the range $\langle -4\,000$ rpm, $4\,000$ rpm \rangle . The normalized control signal in the range $\langle -1, 1 \rangle$ represented control voltage in the range $\langle -10 V, 10 V \rangle$. It should be also noted that no a priori information about the controlled system was used in all control courses presented in this paper and therefore oscillations occur at the beginning of control process where the model does not represent the controlled system well. Performance of individual controllers was tested using summing criteria based on squares and on absolute values of both control error sequence and control sequence differences.

$$S_{e2} = \frac{1}{N_2 - N_1 + 1} \sum_{k=N_1}^{N_2} \left[e(k) \right]^2$$

$$S_{du2} = \frac{1}{N_2 - N_1} \sum_{k=N_1}^{N_2 - 1} \left[u(k+1) - u(k) \right]^2$$

$$S_{ea} = \frac{1}{N_2 - N_1 + 1} \sum_{k=N_1}^{N_2} \left| e(k) \right|$$

$$S_{dua} = \frac{1}{N_2 - N_1} \sum_{k=N_1}^{N_2 - 1} \left| u(k+1) - u(k) \right|$$
(7)

The values of N_1 and N_2 were set to cover whole control process except first 5 s – i.e. the time range for computation of summing criteria was $\langle 5 s, 80 s \rangle$.

Influence of penalisation

The first parameter, which was studied, was penalisation weight λ . Resulting criteria values are presented in Table 1. The sample period $T_0=0.05$ s was used and default values of all other parameters were applied.

Table 1: Influence of the Penalisation

λ	$S_{e2} [10^3]$	$S_{du2}[1]$	$S_{ea}[1]$	<i>S</i> _{dua} [1]
10-6	124.13	0.6779	41.5446	0.2329
0.002	124.12	0.6687	41.8897	0.2387
0.01	124.22	0.6658	41.6476	0.2268
0.04	124.51	0.5445	40.5928	0.1723
0.2	125.97	0.3525	42.4119	0.1328
1	135.04	0.2664	46.8386	0.1001
2	153.18	0.1576	57.9602	0.0682
5	187.05	0.0815	76.1243	0.0518
20	246.90	0.0415	103.6711	0.0387
100	356.24	0.0418	141.6785	0.0545

To simplify comparison of individual settings, criterion values were normalised and values related to quadratic criteria were summed as well as values related to absolute values

$$S_{2}(i) = \frac{1}{2} \left[\frac{S_{e2}(i)}{S_{e2}(nom)} + \frac{S_{du2}(i)}{S_{du2}(nom)} \right]$$

$$S_{a}(i) = \frac{1}{2} \left[\frac{S_{ea}(i)}{S_{ea}(nom)} + \frac{S_{dua}(i)}{S_{dua}(nom)} \right]$$
(8)

The index *nom* in equation (8) represents the values achieved by the nominal controller – i.e. pp2lq controller with sample time $T_0=0.05$, penalisation $\lambda=5$, on-line identification with adaptive directional forgetting and not using a priori information. Values of the S_2 and S_a based on Table 1 are summed up in Table 2.

Table 2: Normalized Criteria for Different Penalisations

λ	S ₂ [1]	S _a [1]
10-6	4.4927	2.5217
0.002	4.4367	2.5798
0.01	4.4188	2.4632
0.04	3.6752	1.9306
0.2	2.5007	1.5610
1	1.9960	1.2738
2	1.3769	1.0393
5	1.0000	1.0000
20	0.9144	1.0546
100	1.2086	1.4565

It is possible to present the values from Table 2 in a graphical form as shown in Fig. 5.



Figure 5: S_2 and S_a Criteria for pp2lq with Different λ

The nominal settings of the *pp2lq* controller are marked by circle. The optimal value of the λ parameter were λ =20 (S_2 criterion) and λ =5 (S_a criterion).

Influence of sample time

The same technique as described in the previous subchapter was used to study the influence of the sample time. The penalization λ =5 was used and all the other parameters remained on their nominal values. Resulting criteria values are summarized in Table 3.

Table 3: Influence of Sample Time

T_0	$S_{2}[1]$	$S_{a}[1]$
0.005	1.1218	2.2919
0.01	0.6886	1.6190
0.025	0.6739	1.0115
0.05	1.0000	1.0000
0.1	1.6034	1.3025
0.2	3.1799	2.9034

The values from the Table 3 are presented in Fig. 6. Optimal value of sample time $T_0=0.025$ s was obtained according to S_2 criterion and $T_0=0.05$ s according to S_a criterion.



Figure 6: S_2 and S_a Criteria for pp2lq with Different T_0

The control courses of $T_0=0.025$ s are presented in Fig. 7.



Figure 7: Control Courses of pp2lq, $T_0=0.025s$

It can be seen that tracking performance of the control system has increased comparing to sample time $T_0=0.05$ (see Fig. 4). On the other hand, greater changes of control signal occurred at the moments of set-point changes.

Influence of forgetting

The last series of experiments performed entirely using *pp2lq* controller was focused on the influence of forgetting to the control process. The problem was studied using exponential forgetting where the forgetting coefficient φ was being changed in the range $\langle 0.6, 1 \rangle$. Resulting criteria values are summarized in Table 4, nominal case using adaptive directional forgetting (*adf*) is also included.

Table 4: Influence of Forgetting Coefficient

arphi	$S_{2}[1]$	$S_{a}[1]$
0.6	3.6062	2.3817
0.7	1.5174	1.2230
0.8	0.9720	0.8354
0.9	0.9654	0.8679
0.95	0.9795	0.9880
0.98	1.1373	1.2870
1	1.5944	2.8767
adf	1.0000	1.0000

The courses of criteria values from the Table 4 are presented in Fig. 8.



Figure 8: S_2 and S_a Criteria for pp2lq with Different φ

The values corresponding to nominal settings with adaptive directional forgetting are represented by the dashed line. Optimal value of forgetting coefficient according to S2 criterion is $\varphi=0.9$. According to Sa criterion, the optimal value $\varphi=0.8$ was obtained.

The value of $\varphi=1$ represents the situation where the weights of all data pairs are the same and therefore exponential forgetting is transformed to pure recursive least squares method (RLSM). On-line identification does not reach satisfactory performance and tracking of the reference signal was not achieved as can be from the control courses presented in Fig. 9.



Figure 9: Control Courses of pp2lq Using Pure RLSM

Influence of control algorithm

The control algorithm plays the most important role when comparing different controllers and their settings. The algorithm is used to compute controller parameters from the current estimates of the parameters of the controlled system model and subsequently compute control sequence. This subchapter contains comparison of several control algorithms from the STCSL. The nominal sample time of T_0 =0.05s and adaptive directional forgetting were used in all cases. The other parameters as well as the values of S_2 and S_a are shown in Table 5.

 Table 5: Performance of Different Control Algorithms

algorithm	$S_{2}[1]$	$S_{a}[1]$	parameters
db2s	4.5380	2.4122	
mv2	1.8083	4.3959	<i>q</i> =10
pp2a_1	1.4491	1.2384	<i>ζ</i> =1, <i>ω</i> =2
pp2b_1	1.6135	1.8294	$\xi=1, \omega=2$
pp2lq	1.0000	1.0000	$\lambda = 5$
zn2ast	4.2882	2.3397	
zn2br	8.4320	3.2525	
zn2pi	4.4683	3.4840	
zn2tak	1.3598	1.0815	
zn3tak	1.4491	1.2384	

Graphical representation of performance of individual control algorithms is expressed in Fig 10.



Figure 10: S₂ and S_a Criteria for Different Algorithms

The db2s is a dead-beat controller. The mv2 is a minimum variance controller, where q is a penalisation coefficient. Controllers $pp2a_1$ and $pp2b_1$ are poleplacement controllers of the one degree of freedom structure and two degree of freedom structure respectively. Positions of the closed loop poles are computed to obtain a dynamic behaviour of the closed loop similar to the second order continuous system with characteristic polynomial

$$d(s) = s^2 + 2\xi\omega s + \omega^2 \tag{10}$$

The *pp2lq* is the nominal LQ controller. The remaining controllers are based on Ziegler-Nichols tuning method.

The *zn2ast* is the Åström controller. The *zn2br* is a Ziegler-Nichols controller with backward rectangular method of integration. The *zn2pi* is a Ziegler-Nichols PI controller. The *zn2tak* and the *z3tak* represent Takahashi's modification of the Ziegler-Nichols algorithm using second and third order model respectively.

The best performance was reached by the nominal pp2lq controller but good results were achieved also by $pp2a_1$ pole-placement controller and by Takahashi's controllers. The control courses of the zn2tak controller are presented in the Fig. 11.



Figure 11: Control Courses of zn2tak controller

Tuning of the *pp2a_1* controller

As can be seen from Table 5, a very good control performance was achieved by the $pp2a_1$ controller. Different settings of parameters ξ and ω were investigated and the results are summarized in Table 6. The sample time of T_0 =0.05s and the adaptive directional forgetting identification method was used in all cases. The nominal pp2lq controller is presented for the comparison purposes.

Table 6: Comparison of Different Settings of pp2a 1

ξ	ω	$S_{2}[1]$	$S_{a}[1]$
0.5	2	2.5086	3.8248
0.8	2	3.7334	2.3190
1	1	15.2416	11.3481
1	2	1.4491	1.2384
1	5	6.2797	1.7654
1	10	6.0036	1.7932
1.5	2	3.3655	1.9910
2	1	7.5373	8.4371
2	2	3.5361	2.2033
nominal J	$pp2lq (\lambda = 5)$	1.0000	1.0000

The best performance was reached by $\xi=1$ and $\omega=2$ according to both S_2 and S_a criteria. The control courses for the $\xi=1$ and $\omega=2$ setting are presented in Fig. 12.



Figure 12: Control Courses of pp2a 1 ($\xi=1, \omega=2$)

CONCLUSIONS

Self-Tuning Controllers Simulink Library was introduced in the paper and controllers from this library were verified in the real-time conditions. Many controllers from the STCSL were tested by control of the Amira DR300 Servo System. This system in nonlinear and contains significant hysteresis.

The goal of the experiments was to find out optimal setting of individual controller algorithms. A set of tested parameters include sample time, control algorithm, forgetting of identification part and others. A convex behaviour was observed for all tested parameters which can be set continuously. Thus, an optimal value of the parameter can be found and change from this optimal setting leads to monotonous increase of a performance criteria. It should be noted that the problem of finding optimal setting of controller parameters is multidimensional, i.e. if other controller parameter changes, the optimal value of the investigated parameter can also change.

The best performance was achieved by LQ controller but satisfactory results were also produced by simpler Ziegler-Nichols based controllers.

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SIMULATION OF ADAPTIVE CONTROL OF A CONTINUOUS STIRRED TANK REACTOR

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KEYWORDS

Simulation, adaptive control, continuous-time linear model, delta model, parameter estimation, polynomial method.

ABSTRACT

The paper deals with simulation of continuous-time adaptive control of a continuous stirred tank reactor (CSTR). The control design is based on approximation of a nonlinear model of the process by a continuoustime external linear model.with parameters estimated using a corresponding delta model. The control system with two feedback controllers is considered. The controller design is based on the polynomial approach and the pole assignment method. The adaptive control is tested by simulations on the nonlinear model of the CSTR with a consecutive exothermic reaction.

INTRODUCTION

Continuous stirred tank reactors (CSTRs) belong to a class of nonlinear systems where both steady-state and dynamic behaviour are nonlinear. Their models are derived and described in e.g. (Ogunnaike and Ray 1994; Schmidt 2005; Corriou 2004). The process nonlinearities may cause difficulties when controlling using conventional controllers with fixed parameters. One possible method to cope with this problem is using adaptive strategies based on an appropriate choice of an external linear model (ELM) with recursively estimated parameters. These parameters are consequently used for parallel updating of controller's parameters.

The control itself can be either continuous-time or discrete. Experiences of authors in the field of control of nonlinear technological processes indicate that the continuous- time (CT) approach gives better results when controlling processes with strong nonlinearities.

For the CT ELM parameters estimation, either the direct method or application of an external delta model with the same structure as the CT model can be used (Dostál et al. 2004). In this paper, an approach based on the delta model was applied.

The basics of delta models have been described in e.g. (Middleton and Goodwin 1990; Mukhopadhyay et al. 1992; Goodwin et al. 2001). Although delta models belong into discrete models, they do not have such disadvantages connected with shortening of a sampling

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) period as discrete z-models. In addition, parameters of delta models can directly be estimated from sampled signals. Moreover, it can be easily proved that these parameters converge to parameters of CT models for a sufficiently small sampling period (compared to the dynamics of the controlled process). Complete description and experimental verification can be found in (Stericker and Sinha 1993).

This contribution presents in brief a procedure of a CSTR control design and, consequently, the control simulation results. The parameters of the CT ELM are obtained via corresponding delta model parameter estimation. The control system with two feedback controllers is used according to (Ortega and Kelly 1984; Dostál et al. 2007). This set-up gives better control results for the reference tracking than the use of only a feedback controller. Input signals for the control system are considered as step functions. The resulting continuous-time controllers derived using polynomial and pole assignment methods (Kučera 1993) guarantee stability of the control system, asymptotic tracking of step references and step load disturbances attenuation. The simulations are performed on a nonlinear model of the CSTR with a consecutive exothermic reaction.

MODEL OF THE PLANT

Consider a CSTR with the first order consecutive exothermic reaction according to the scheme $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ and with a perfectly mixed cooling jacket. Using the usual simplifications, the model of the CSTR is described by four nonlinear differential equations

$$\frac{dc_A}{dt} = -\left(\frac{Q_r}{V_r} + k_1\right)c_A + \frac{Q_r}{V_r}c_{Af}$$
(1)

$$\frac{dc_B}{dt} = -\left(\frac{Q_r}{V_r} + k_2\right)c_B + k_1c_A + \frac{Q_r}{V_r}c_{Bf}$$
(2)

$$\frac{dT_r}{dt} = \frac{h_r}{(\rho c_p)_r} + \frac{Q_r}{V_r} (T_{rf} - T_r) + \frac{A_h U}{V_r (\rho c_p)_r} (T_c - T_r)$$
(3)

$$\frac{dT_c}{dt} = \frac{Q_c}{V_c} (T_{cf} - T_c) + \frac{A_h U}{V_c (\rho c_p)_c} (T_r - T_c)$$
(4)

with initial conditions $c_A(0) = c_A^s$, $c_B(0) = c_B^s$, $T_r(0) = T_r^s$ and $T_c(0) = T_c^s$. Here, t is the time, c are concentrations, T are temperatures, V are volumes, ρ are densities, c_p are specific heat capacities, Q are volumetric flow rates, A_h is the heat exchange surface area and U is the heat transfer coefficient. The subscripts are denoted (γ_r for the reactant mixture, (γ_c for the coolant, (γ_f for feed (inlet) values and the superscript (γ_s for steady-state values. The reaction rates and the reaction heat are expressed as

$$k_j = k_{0j} \exp\left(\frac{-E_j}{RT_r}\right), \ j = 1, 2$$
(5)

$$Q_{r} = (-\Delta H_{r1})k_{1}c_{A} + (-\Delta H_{r2})k_{2}c_{B}$$
(7)

where k_0 are pre-exponential factors, *E* are activation energies and $(-\Delta H_r)$ are in the negative considered reaction entalpies. The values of all parameters, feed values and steady-state values in the operating point (initial conditions for (1) - (4)) are given in Table 1.

Table 1. Parameters, inlet values and initial conditions

$Q_{\rm r}^{\rm s} = 0.08 {\rm m}^3 {\rm min}^{-1}$
$Q_{\rm c}^{\rm s} = 0.073 {\rm m}^3 {\rm min}^{-1}$
$c_{\rm pr} = 4.05 \text{ kJ kg}^{-1} \text{K}^{-1}$
$c_{\rm pc} = 4.18 \text{ kJ kg}^{-1} \text{K}^{-1}$
$U = 43.5 \text{ kJ m}^{-2} \text{min}^{-1} \text{K}^{-1}$
$E_1/R = 13477 \text{ K}$
$E_2/R = 15290 \text{ K}$
$(-\Delta H_{R2}) = 2.2 \cdot 10^4 \text{kJ kmol}^{-1}$
$c_{\rm Bf} = 0 \text{ kmol m}^{-3}$
$T_{\rm cf} = 293 \; {\rm K}$
$c_{\rm b}^{\rm s} = 1.361 \text{ kmol m}^{-3}$
$T_{\rm c}^{\rm s} = 308.0 {\rm K}$

In term of the practice, only the coolant flow rate can be taken into account as the control input. On behalf of selection of a suitable controlled output, the dynamic charakteristics were computed in the neighbourhood of the operating point. The input and both outputs were considered as deviations from steady values. The deviations are denoted as follows:

$$\Delta Q_c = Q_c(t) - Q_c^s, \qquad \Delta c_B(t) = c_B(t) - c_B^s$$

 $\Delta T_r(t) = T_r(t) - T_r^s$ The responses in Figs. 1 and 2 show a better applicability of the reactant temperature as the controlled output in comparison with the component B output concentration having in this regard very unfavourable properties.

CT AND DELTA EXTERNAL LINEAR MODEL

For the control purposes, the controlled output and the control input were defined as

$$y(t) = \Delta T_r(t) = T_r(t) - T_r^s$$
, $u(t) = 10 \frac{Q_c(t) - Q_c^s}{Q_c^s}$. (7)



Figure 1: Component B output concentration step responses.



Figure 2: Reactant temperature step responses.

These expressions enable to obtain variables of approximately the same magnitude.

Taking into account curves in Fig. 2, the second order CT ELM can be chosen in the form of the second order linear differential equation

$$\ddot{y}(t) + a_1 \dot{y}(t) + a_0 y(t) = b_1 \dot{u}(t) + b_0 u(t)$$
(8)

or, in the transfer function representation as

$$G(s) = \frac{b_1 s + b_0}{s^2 + a_1 s + a_0}.$$
 (9)

Establishing the δ operator

$$\delta = \frac{q-1}{T_0} \tag{10}$$

where q is the forward shift operator and T_0 is the sampling period, the delta ELM corresponding to (8) takes the form

$$\delta^2 y(t') + a'_1 \delta y(t') + a'_0 y(t') = b'_1 \delta u(t') + b'_0 u(t') (11)$$

where t' is the discrete time.

When the sampling period is shortened, the delta operator approaches the derivative operator, and, the estimated parameters a',b' reach the parameters a, b of the CT model as shown in (Stericker and Sinha 1993).

DELTA MODEL PARAMETER ESTIMATION

Substituting t' = k - 2, equation (11) may be rewriten to the form

$$\delta^{2} y(k-2) + a'_{1} \delta y(k-2) + a'_{0} y(k-2) =$$

= b'_{1} \delta u(k-2) + b'_{0} u(k-2) (12)

Establishing the regression vector

$$\boldsymbol{\Phi}_{\delta}^{T}(k-1) = \left(\delta y(k-2) \ y(k-2) \\ \delta u(k-2) \ u(k-2)\right)$$
(13)

where

$$\delta y(k-2) = \frac{y(k-1) - y(k-2)}{T_0}$$
$$\delta u(k-2) = \frac{u(k-1) - u(k-2)}{T_0},$$

the vector of delta model parameters

$$\boldsymbol{\Theta}_{\delta}^{T}(k) = \left(a_{1}^{\prime} a_{0}^{\prime} b_{1}^{\prime} b_{0}^{\prime}\right)$$
(14)

is recursively estimated from the equation

$$\delta^2 y(k-2) = \boldsymbol{\Theta}_{\delta}^T(k) \boldsymbol{\Phi}_{\delta}(k-1) + \varepsilon(k)$$
(15)

where

$$\delta^2 y(k-2) = \frac{y(k) - 2y(k-1) + y(k-2)}{T_0^2}.$$
 (16)

The recursive estimation of delta model parameters was performed with the sampling interval $T_0 = 0.5$ min. Here, the recursive identification method with exponential and directional forgetting according to (Rao and Unbehauen 2005; Bobál et al. 2005) was used.

CONTROL SYSTEM DESCRIPTION

The control system with two feedback controllers is depicted in Fig. 3. In the scheme, w is the reference signal, v denotes the load disturbance, e is the tracking error, u_0 is the output of the controller, y is the controlled output and u is the control input.



Figure 3: Control system with two feedback controllers.

In general therms, G represents the ELM with the transfer function

$$G(s) = \frac{b(s)}{a(s)} \tag{17}$$

and Q and R are feedback controllers with transfer functions

$$Q(s) = \frac{\widetilde{q}(s)}{\widetilde{p}(s)}, \quad R(s) = \frac{r(s)}{\widetilde{p}(s)}$$
(18)

where \tilde{q} , r and \tilde{p} are polynomials in s.

Both w and v are considered to be step functions with transforms

$$W(s) = \frac{w_0}{s}, V(s) = \frac{v_0}{s}.$$
 (19)

APPLICATION OF POLYNOMIAL METHOD

The controller design described in this section appears from the polynomial approach. General conditions required to govern the control system properties are formulated as strong stability (in addition to the control system stability, also the stability of controllers is required), internal properness, asymptotic tracking of the reference and load disturbance attenuation.

The procedure to obtain admissible controllers can be briefly described as follows: Establish the polynomial t as

$$t(s) = r(s) + \tilde{q}(s) .$$
⁽²⁰⁾

Then, the control system stability is ensured when polynomials \tilde{p} and *t* are given by a solution of the polynomial Diophantine equation

$$a(s)\widetilde{p}(s) + b(s)t(s) = d(s)$$
(21)

with a stable polynomial d on the right side. Evidently, the roots of d determine poles of the closed-loop.

Further, the asymptotic tracking and load disturbance attenuation are provided by polynomials \tilde{p} and \tilde{q} having the form

$$\tilde{p}(s) = s \ p(s), \quad \tilde{q}(s) = s \ q(s) \ . \tag{22}$$

Subsequently, the transfer functions of controllers take forms

$$Q(s) = \frac{q(s)}{p(s)}, \quad R(s) = \frac{r(s)}{s p(s)}.$$
 (23)

A stable polynomial p(s) in denominators of (23) ensures the stability of controllers.

The control system satisfies the condition of internal properness when the transfer functions of all its components are proper. Consequently, the degrees of polynomials q and r must fulfill inequalities

$$\deg q \le \deg p , \ \deg r \le \deg p + 1 .$$
 (24)

Now, the polynomial *t* can be rewritten into the form

$$t(s) = r(s) + s q(s)$$
. (25)

Taking into account solvability of (21) and conditions (24), the degrees of polynomials in (21) and (24) can be easily derived as

$$\deg t = \deg r = \deg a , \ \deg q = \deg a - 1 ,$$

$$\deg p \ge \deg a - 1, \ \deg d \ge 2 \deg a.$$
 (26)

Denoting deg a = n, polynomials t, r and q have forms

$$t(s) = \sum_{i=0}^{n} t_i s^i , \ r(s) = \sum_{i=0}^{n} r_i s^i , \ q(s) = \sum_{i=1}^{n} q_i s^{i-1}$$
(27)

where their coefficients fulfill equalities

$$r_0 = t_0, \quad r_i + q_i = t_i \text{ for } i = 1, \dots, n$$
 (28)

Then, unknown coefficients r_i and q_i can be obtained by a choice of selectable coefficients $\beta_i \in \langle 0, 1 \rangle$ such that

$$r_i = \beta_i t_i, \quad q_i = (1 - \beta_i) t_i \text{ for } i = 1, ..., n.$$
 (29)

The coefficients β_i split a weight between numerators of transfer functions Q and R. With respect to (23) and (29), it may be expected that higher values of β_i will speed up control responses to step references.

Remark: If $\beta_i = 1$ for all *i*, the control system in Fig. 1 simplifies to the 1DOF control configuration. If $\beta_i = 0$ for all *i* and both reference and load disturbance are step functions, the control system corresponds to the 2DOF control configuration.

The controller parameters then follow from solution of the polynomial equation (21) and depend upon coefficients of the polynomial d.

Now, for the second order model (9) with deg a = 2, the numerators in (23) take forms

$$q(s) = q_2 s + q_1, \quad r(s) = r_2 s^2 + r_1 s + r_0$$
 (30)

where

$$r_1 = \beta_1 t_1, \ r_2 = \beta_2 t_2, q_1 = (1 - \beta_1) t_1, \ q_2 = (1 - \beta_2) t_2.$$
(31)

POLE ASSIGNMENT

A required control quality can be achieved by a suitable determination of the polynomial d on the right side of (21).

In this paper, the polynomial d is chosen as a product of two stable factors

$$d(s) = g(s) n(s) . \tag{32}$$

Here, g is the third order stable polynomial

$$g(s) = g_3 s^3 + g_2 s^2 + g_1 s + g_0$$
(33)

given by spectral factorization

$$[s a(s)]^* \varphi[s a(s)] + b^*(s)b(s) = g^*(s)g(s) \quad (34)$$

and asterisk denotes a conjugate polynomial.

Note that the spectral factorization (34) is well known from the LQ control theory. There *g* appears from a claim of minimization of the cost function

$$J = \int_{0}^{\infty} \left[e^2(t) + \varphi \dot{u}^2(t) \right] dt$$
 (35)

where ϕ is the weight coefficient.

The polynomial *n* is the second order stable polynomial

$$n(s) = s^2 + n_1 s + n_0 \tag{36}$$

resulting from spectral factorization

$$n^{*}(s)n(s) = a^{*}(s)a(s)$$
 (37)

The form (32) leads to strictly proper controllers with transfer functions

$$Q(s) = \frac{q_2 s + q_1}{s^2 + p_1 s + p_0}, \quad R(s) = \frac{r_2 s^2 + r_1 s + r_0}{s (s^2 + p_1 s + p_0)}.$$
 (38)

Note that the choice of d in the form (32) provides the control of a good quality for aperiodic controlled processes.

Now, it follows from the above introduced procedure that the parameters of both controllers depend upon coefficients β as well as upon the parameter ϕ which affects the closed-loop poles. Consequently, tuning of the controllers can be performed by a suitable choice of selectable parameters β and ϕ .

The adaptive control system is shown in Fig. 4.



Figure 4: Adaptive control with delta ELM parameter estimation.

SIMULATION RESULTS

For the start (the adaptation phase), a P controller with a small gain was used in all simulations.

The effect of the parameter φ on the control responses in the 1DOF structure is transparent from Figs. 5 and 6. Here, three values φ were selected. The control results show sensitivity of the controlled output and control input to φ . An decreasing φ leads to overshoots of the controlled output and higher values and changes of the control input.

The control responses for $\beta_1 = \beta_2 = 1$ (the 1DOF structure), $\beta_1 = \beta_2 = 0.5$ and $\beta_1 = \beta_2 = 0$ (the 2DOF structure) with the same φ are compared in Figs. 7 and 8. The presented results show that by a suitable choice of parameters β , the control responses of a good quality can be achieved. Moreover, decreasing values β lead to smaller control input changes. This fact can be important for a practical control where greater input changes may be undesirable.

The simulated control responses for $\beta_2 = 0$ and different values β_1 are shown in Figs. 9 and 10. The effect of the parameter β_1 is evident. Its increase speeds up the control, but, it can lead to overshoots of the controlled output and to higher control input changes (derivatives). The presence of the integrating part in the controller Renables not only attenuation of a step disturbance loaded on *u*, but also rejection of other step disturbances entering into the process. Here, step disturbances in the component A inlet concentration $v(t) = \Delta c_{Af}(t) = \pm 0.142 \text{ kmol m}^{-3}$ at times $t_v = 200 \text{ min and } t_v = 350 \text{ min are considered.}$ The controller parameters were estimated only in the first (tracking) interval t < 190 min. During interval $t \ge$ 190 min, fixed parameters were used.

The disturbances and controlled output responses are shown in Fig. 11.



Figure 5: Controlled outputs for various φ (1DOF).





Figure 7: Controlled outputs for various β_1 , β_2 ($\phi = 1$).



Figure 8: Control inputs for various β_1 , β_2 ($\phi = 1$).



Figure 9: Controlled outputs for various β_1 ($\phi = 1$).



Figure 10: Control inputs for various β_1 ($\phi = 1$).



Figure 11: Step disturbance attenuation (1DOF, $\phi = 1$).

CONCLUSIONS

An objective of the article was to verify by simulations an adapteve control algorithm derived for a continuous stirred tank reactor. The presented strategy uses two feedback controllers and enables to create an effective control algorithm. This algorithm is based on an alternative continuous-time external linear model with parameters obtained through recursive parameter estimation of a corresponding delta model. Both resulting continuous-time controllers are derived using the polynomial approach and given by a solution of a polynomial Diophantine equation. Tuning of their parameters is possible either via the parameter affecting the closed-loop poles or by a choice of selectable coefficients splitting a weight between numerators of controllers' transfer functions. The presented method has been tested by computer simulation on the nonlinear model of the CSTR with a consecutive exothermic reaction. The results demonstrate the applicability of the presented control strategy.

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RELAY-BASED AUTOTUNING WITH ALGEBRAIC CONTROL DESIGN

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KEYWORDS

Autotuning, Algebraic control design, Pole-placement problem, PID controller, Relay.

ABSTRACT

In this paper, a combination of relay feedback identification and an algebraic control design method for stable systems is studied. Models with up to three parameters are estimated by means of a single asymmetrical relay experiment. Then a stable low order transfer function is identified. Then the controller is analytically derived from general solutions of Diophantine equations in the ring of proper and stable rational functions. The controller parameters are tuned through a pole-placement problem as a desired multiple root of the characteristic closed loop equation. A first order identification yields a PI-like controllers while a second order identification generates PID ones. The approach enables a scalar tuning parameter m>0 which can be adjusted by various principles.

INTRODUCTION

Since industrial processes are usually complex and nonlinear the task to control their loops properly becomes difficult and challenging. Moreover, the majority of controllers used in industrial applications have been still of the PID type. The practical advantages of PID controllers can be seen in a simple structure, in an understandable principle and in control capabilities. It is widely known that PID controllers are quite resistant to changes in the controlled process without meaningful deterioration of the loop behavior. A solution for qualified choice of controller parameters can be seen in automatic tuning of PID controllers.

The development of various autotuning principles was started by a simple symmetrical relay feedback experiment proposed by Åström and Hägglund, 1984. The ultimate gain and ultimate frequency are then used for adjusting of parameters by common known Ziegler-Nichols rules. During the period of more than two decades, many studies have been reported to extend and improve autotuners principles; see e.g. (Åströn and Hägglung, 1995; Ingimundarson and Hägglund, 2000; Majhi and Atherton, 1998; Morilla and Gonzáles, 2000). The extension in an experimental phase was performed in (Yu, 1999; Pecharromán and Pagola, 2000; Kaya and Atherton, 2001) by an asymmetry and hysteresis of a relay, see (Thyagarajan and Yu, 2002; Kaya and Atherton, 2001), and experiments with asymmetrical and dead-zone relay feedback are reported in (Vítečková and Víteček, 2004; Vyhlídal, 2000). Also, various control design principles and rules can be investigated in mentioned references. Nowadays, almost all commercial industrial PID controllers provide the feature of autotuning.

This paper is focused on a novel combination for autotunig method of PI and PID controllers. The method combines an asymmetrical relay identification experiment and a control design method which is based on a pole-placement principle. The pole placement problem is formulated through a Diophantine equation and it is tuned by an equalization setting proposed in (Gorez and Klán, 2000).

RELAY FEEDBACK ESTIMATION

The estimation of the process or ultimate parameters is a crucial point in all autotuning principles. The relay feedback test can utilize various types of relay for the parameter estimation procedure. The classical relay feedback test (Åström and Hägglund, 1984) proposed for stable processes a symmetrical relay without hysteresis. Then the critical (ultimate) values can be estimated and a control design can follow.

Asymmetrical relays with or without hysteresis bring further progress (Yu, 1999; Kaya and Atherton, 2001). After the relay feedback test, the estimation of process parameters can be performed. A typical data response of such relay experiment is depicted in Figure 1. The relay asymmetry is required for the process gain estimation (2) while a symmetrical relay would cause the zero division in the appropriate formula.

In this paper, an asymmetrical relay with hysteresis was used. This relay enables to estimate transfer function parameters as well as a time delay term. For the purpose of this contribution the time delay was not utilized.

The model for first order (stable) systems plus dead time (FOPDT) is supposed in the form:

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$$G(s) = \frac{K}{Ts+1} \cdot e^{-\Theta s} \tag{1}$$

and the process gain can be computed by the relation (Vyhlídal, 2000):

$$K = \frac{\int_{0}^{iT_{i}} y(t)dt}{\int_{0}^{iT_{i}} u(t)dt}; \quad i = 1, 2, 3, \dots$$
(2)



Figure 1: Asymmetrical relay oscillation of stable process

The time constant and time delay terms are given by (Vítečková and Víteček, 2004):

$$T = \frac{T_{y}}{2\pi} \cdot \sqrt{\frac{16 \cdot K^{2} \cdot u_{0}^{2}}{\pi^{2} \cdot a_{y}^{2}} - 1}}$$

$$\Theta = \frac{T_{y}}{2\pi} \cdot \left[\pi - \arctan \frac{2\pi T}{T_{y}} - \arctan \frac{\varepsilon}{\sqrt{a_{y}^{2} - \varepsilon^{2}}} \right]$$
(3)

where a_y and T_y are depicted in Fig.1 and ε is hysteresis.

Similarly, the second order model plus dead time (SOPDT) is assumed in the form:

$$G(s) = \frac{K}{\left(Ts+1\right)^2} \cdot e^{-\Theta s} \tag{4}$$

The gain is given by (2), the time constant and time delay term can be estimated according to (Vítečková and Víteček, 2004) by the relation:

$$T = \frac{T_{y}}{2\pi} \cdot \sqrt{\frac{4 \cdot K \cdot u_{0}}{\pi \cdot a_{y}} - 1}$$

$$\Theta = \frac{T_{y}}{2\pi} \cdot \left[\pi - 2 \operatorname{arctg} \frac{2\pi T}{T_{y}} - \operatorname{arctg} \frac{\varepsilon}{\sqrt{a_{y}^{2} - \varepsilon^{2}}} \right]$$
(5)

ALGEBRAIC CONTROLLER DESIGN

The control design is based on the fractional approach; see e.g. (Vidyasagar, 1987; Kučera, 1993; Prokop and Corriou, 1997; Prokop, et al., 2002). Any transfer function G(s) of a (continuous-time) linear system is expressed as a ratio of two elements of R_{PS} . The set R_{PS} means the ring of (Hurwitz) stable and proper rational functions. Traditional transfer functions as a ratio of two polynomials can be easily transformed into the fractional form simply by dividing, both the polynomial denominator and numerator by the same stable polynomial of the order of the original denominator. Then all transfer functions can be expressed by the ratio:

$$G(s) = \frac{b(s)}{a(s)} = \frac{\frac{b(s)}{(s+m)^{n}}}{\frac{a(s)}{(s+m)^{n}}} = \frac{B(s)}{A(s)}$$
(6)

$$n = \max(\deg(a), \deg(b)), \quad m > 0 \tag{7}$$

Then all feedback stabilizing controllers according to Figure 2 are given by a general solution of the Diophantine equation:

$$AP + BQ = 1 \tag{8}$$

which can be expressed with Z free in R_{PS} :

$$\frac{Q}{P} = \frac{Q_0 - AZ}{P_0 + BZ} \tag{9}$$



Figure 2: Feedback (1DOF) control loop

Asymptotic tracking is then ensured by the divisibility of the denominator P in (9) by the denominator of the reference $w = \frac{G}{F}$ which is supposed in the form:

$$F_{w} = \frac{s}{s+m}; \quad m > 0 \tag{10}$$

The set of reference signals with denominator (10) represents all stepwise signals which are most frequent references. The divisibility is achieved by a suitable choice of rational function Z in (9), see (Prokop, et al., 2002).

PI AND PID-LIKE CONTROLLERS

The control design for first order systems (1) gives the Diophantine equation (8) in the form:

$$(Ts+1)p_0 + Kq_0 = s + m \tag{11}$$

and the general solution is given by:

$$P = \frac{1}{T} + \frac{K}{s+m} \cdot Z$$

$$Q = \frac{Tm-1}{TK} - \frac{Ts+1}{s+m} \cdot Z$$
(12)

where Z is free in the ring R_{PS} . Asymptotic tracking is achieved by the choice:

$$Z = -\frac{m}{TK}$$
(13)

and the resulting PI controller is in the form:

$$C(s) = \frac{Q}{P} = \frac{q_1 s + q_0}{s}$$
(14)

where parameters q_1 a q_0 are given by:

$$q_1 = \frac{2Tm - 1}{K} \qquad q_0 = \frac{Tm^2}{K}$$
 (15)

For the SOPDT the design equation takes the form:

$$(Ts+1)^{2} \cdot s \cdot p_{0} + K \cdot (q_{2}s^{2} + q_{1}s + q_{0}) = (s+m)^{3}$$
(16)

and after similar manipulations the resulting PID controller gives the transfer function:

$$C(s) = \frac{Q}{P} = \frac{q_2 s^2 + q_1 s + q_0}{s(s + p_0)}$$
(17)

with parameters:

$$p_{0} = \frac{1}{T^{2}}; \qquad q_{2} = \frac{3Tm - 2}{KT}$$

$$q_{1} = \frac{3T^{2}m^{2} - 1}{KT^{2}}; \qquad q_{0} = \frac{m^{3}}{K}$$
(18)

For both systems FOPDT and SOPDT the scalar parameter m>0 seems to be a suitable "tuning knob" influencing control behavior as well as robustness properties of the closed loop system.

The control law for the equalization method (Gorez and Klán, 2000) is supposed in the form of the PI controller:

$$u(t) = K_{P} \cdot \left(e(t) + \frac{1}{T_{I}} \cdot \int e(\tau) d\tau \right)$$
(19)

The PI controller parameters can be tuned by simple relations:

$$K_{p} = \frac{1}{2K} \qquad T_{I} = 0.4 \cdot T_{u} \tag{20}$$

where K is process gain and T_u is ultimate period.

The parameter q_1 in (15) represents the controller gain and is tuned by the "equalization" principle. The choice for the tuning parameter m>0 in the case of PI controller is given by:

$$m = \frac{3}{4 \cdot T} \tag{21}$$

Naturally, this choice of m does not yield the same value of T_I given by formula (20). However, the difference is not significant and the authors prefer the influence of the controller gain.

EXAMPLES AND ANALYSIS

The following three examples illustrate the situation where the controlled system is always estimated by the first order one (1) with or without time delay terms and the controller has a PI structure (14).

The first order system governed by the transfer function G(s) was after the relay experiment estimated by $\tilde{G}(s)$ in the form:

$$G(s) = \frac{2}{3s+1} \qquad \widetilde{G}(s) = \frac{2}{2.93s+1}$$
(22)



Figure 3: Step responses of nominal and estimated systems

The PI controller was then generated for m=0,256 by relations (14), (15) and the resulting control behavior are depicted in Figure 4.



Figure 5: Control responses for two different values m>0

The choice of the parameter m>0 can easily influence the control response, e.g. the increasing value of m>0accelerate the control response but escalate overshoots. The situation for two values of m>0 is shown in Figure 5.

The next example represents the situation where a second order (stable) system G(s) was estimated by a first order model in the above mentioned relay experiment. Both transfer functions have the form:

$$G(s) = \frac{3}{(2s+1)^2} \quad \widetilde{G}(s) = \frac{3.02}{3.89s+1} \cdot e^{-1.15s}$$
(23)

The PI controller generated from the approximated system $\tilde{G}(s)$ for the scalar tuning parameter m=0.19 and applied to the system G(s) gives the control response depicted in Figure 7.

Comparison of two control responses for two different values of the tuning parameter m can be seen in Figure 8.



Figure 7: Control response for m=0.19 for second order system G in (23)



Figure 8: Control responses of the second order systems for two values m>0

As a third example a high order system with transfer function G(s) was supposed. Again, after the relay experiment, a first order estimation $\widetilde{G}(s)$ was identified, both governed by:

$$G(s) = \frac{3}{(s+1)^8} \qquad \widetilde{G}(s) = \frac{3}{3.52s+1} \cdot e^{-5.2s} \qquad (24)$$

Naturally, the step response of the estimated system is different from the nominal system as depicted in Figure 9 because the time-delay is neglected. However, the control design for m=0.2 gives the PI controller and the resulting control behavior is shown in Figure 10.





Time (s)

Again, the tuning parameter m>0 can influence the control response. Figure 11 illustrates further control behavior for different PI controllers. In all simulations, the reference value is changed in 1/3 of the simulation horizon and the load disturbance is injected in the 2/3 of the simulation horizon.

As a last example, the fourth order controlled system is supposed in the form

$$G(s) = \frac{2}{\left(0.5s + 1\right)^4}$$
(25)

The second order identification relations (5) give the estimated transfer function:

$$\tilde{\tilde{G}}(s) = \frac{2.007}{\left(0.612s + 1\right)^2} \cdot e^{-0.58s}$$
(26)

and Figure 12 shows the original and approximated step responses of (26) with and without the time delay term.





Figure 12: Step responses of systems (25) - (26)

The controller was designed for the estimated transfer function (26) according to SOPDT synthesis (16) – (18). The final control responses for two different tuning parameters m>0 are depicted in Figure 13. Naturally, the controlled system in simulations was the original one in (25). Again, the influence of the scalar tuning parameter is obvious and apparent.



CONCLUSION

This contribution gives a new combination of relay feedback identification and a control design method as an autotuning principle. The estimation of a low order transfer function parameters is performed from asymmetric limit cycle data. The control synthesis is carried out through the solution of a linear Diophantine equation; see (Vidyasagar, 1987; Kučera, 1993; Prokop and Corriou, 1997; Prokop, et al., 2002). This approach brings a scalar tuning parameter which can be adjusted by various strategies. A first order estimated model generates PI-like controllers while a second order model gives a class of PID ones. The methodology is illustrated by several examples of various orders and dynamics.

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SIMULATION-BASED OPTIMIZATION OF MARKOV CONTROLLED PROCESSES WITH UNKNOWN PARAMETERS

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KEYWORDS

Markov Chains, adaptive control, simulation-based optimization, gradient estimation, online algorithms.

Abstract

We consider simulation-based gradient-estimation and its use in Markov controlled processes with unknown parameters. We consider a Markov reward process controlled by both a set of tunable parameters, and a set of fixed but unknown. We analyze the use a recursive identification procedure, and their application to existing gradient-based algorithms based on simulation. We show that simple modifications of available gradient estimation algorithms, namely assuming parameter certainty, can accommodate system parameter identification, without sacrificing the convergence of these to local optima by following a two-time-scale recursive identification/optimization procedure. This approach is illustrated through an application to the algorithm proposed in (Marbach and Tsitsiklis, 2001). We illustrate our results with a small numerical example, which we further use to test the ability of the proposed scheme to track slow changing system parameters.

INTRODUCTION

Many stochastic resource allocation and control problems can be naturally modeled using dynamic programming. Unfortunately, the dynamic programming algorithm suffers from the 'curse of dimensionality'. In order to address these performance problems, researchers have recurred to the use of parameterized control policies, as in (Marbach and Tsitsiklis, 2001), reducing the problem to one of search in policy space. Several simulationbased techniques exist (Marbach and Tsitsiklis, 2001, 2003; Cao and Chen, 1997; Cao and Wan, 1998; Fang and Cao, 2004; Baxter and Bartlett, 2001) that use realizations of the stochastic processes to obtain gradient estimates that can be used in a gradient-based search method in policy space.

Many of the algorithms mentioned above are 'modelfree' and, hence, implicitly adaptive, e.g., general stochastic approximations (Kiefer and Wolfowitz, 1952; Kushner and Yin, 1997), but they exhibit slow convergence due to biased gradient estimates, or large variances. This problem can be alleviated by incorporating knowledge of the system model, for example by exploiting regenerative structure to eliminate bias, but by requiring knowledge of all system parameters, the usefulness of such techniques is limited. Although the problem of adaptive control of Markov chains has been studied before, most of authors address the case of a finite number of possible models, as in (Mandl, 1974; Borkar and Varaiya, 1979; Kumar and Becker, 1982; Doshi, 1980; El-Fattah, 1981). Other authors, overcome this restriction, but assume that the optimal policies for each model can be easily computed, such as in (Borkar and Varaiya, 1982). Others, embed the estimation process in a value iteration procedure (Hernández-Lerma, 1989), which is not efficient computationally when the state spaces are large. The work in (Ren and Krogh, 2001; Santharam and Sastry, 1997) estimates Q-factors, a technique that is adaptive since no system model is in principle needed, but requires the action set to be finite in order to build a Q-factor for each state-action pair, and quickly becomes impractical as the state space increases. In some specific cases, the Q-factors can be approximated via a neural network or other architectures (Bertsekas and Tsitsiklis, 1996), with limited success.

In this paper we consider the problem of adaptive optimization of parameterized Markov reward processes. We first study the problem of online estimation and optimization of the average reward criterion in Markov reward processes for which the transition probabilities, as well as the expected reward per stage, are functions of two sets of parameters: 1) a set of tunable controls, and 2) a fixed but unknown parameter. We study estimation procedures that can be updated after each transition in the chain, generalizing some of the results of (Campos-Nanez and Patek, 2005), apply them to existing simulation-based algorithms, such as the algorithm of (Marbach and Tsitsiklis, 2001), providing sufficient conditions for the convergence of the resulting method to a local optimum.

The paper is organized as follows. We first present the problem of adaptive Markov control, and address the problem of estimation of an unknown parameter. We follow this with a discussion about the use of estimators in

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optimization algorithms, and illustrate our approach using an algorithm developed in (Marbach and Tsitsiklis, 2001). We provide sufficient conditions for the convergence of the adaptive scheme to local optima, while identifying the true system parameter values. The resulting adaptive algorithm has small memory and computational requirements, and can hence be implemented in an fashion. Its performance is discussed in the last section of the paper, where its usability under slow changing parameters is explored.

MARKOV REWARD PROCESSES WITH UN-KNOWN PARAMETERS

Let $\{i_n\}_n$ be a discrete-time Markov chain with finite state space $S = \{1, 2, ..., N\}$. There is a set of 'tunable' parameters $u \in \mathbb{R}^K$, and a fixed but unknown parameter $\theta^* \in \Theta$, a convex, compact subset of \mathbb{R} . These two sets of parameters determine the dynamics of the Markov chain in the sense that the transition probabilities

$$p_{ij}(u, \theta^*) = P(i_{n+1} = j \mid i_n = i, u, \theta^*),$$

are functions of the control vector u, and the parameter θ^* . We define $P(u, \theta^*)$ to be the transition probability matrix with entries $p_{ij}(u, \theta^*)$. The reward observed by this system is also a function of parameters u, and θ^* , i.e., the expected reward per stage when the system is at state *i*, and controls *u* are applied is a function of u, θ^* , denoted by $g_i(u, \theta^*)$.

We focus our attention to the average reward criterion, which can be defined as

$$\lambda(u,\theta^*) = \liminf_{T \to \infty} \frac{1}{T} E\left[\sum_{n=0}^T g_{i_n}(u,\theta^*) \middle| i_0 = i \right], \quad (1)$$

which we want to maximize. We point out that the problem can be thought of as having two parts. On one hand one must estimate the unknown parameter θ^* . On the other, we must select the value for *u* that maximizes $\lambda(u, \theta^*)$. Moreover, it is desirable to solve the two questions simultaneously, in order to construct an adaptive algorithm. Building such algorithms is the focus of this paper, but before we do so, we have to state the following structural assumptions, many of which are common in the adaptive Markov control literature (Borkar and Varaiya, 1979).

Assumption 1. The transition probability matrix $P(u, \theta)$ defines a Markov chain that is irreducible and aperiodic for all values of $u \in \mathbb{R}^{K}$ and $\theta \in \Theta$.

Under this assumption one can conclude that for all $u \in \mathbb{R}^{K}$ and $\theta^{*} \in \Theta$, all states will be recurrent and the steadystate distribution $\pi(u, \theta^{*})$ will exist. Consequently, the limit in (1) exists, is independent of the initial state, and is equal to

$$\lambda(u, \theta^*) = \sum_{i \in S} \pi(u, \theta^*) g_i(u, \theta^*)$$

Assumption 2. The functions $P(u, \theta)$, and $g_i(u, \theta)$ are assumed to be twice differentiable with bounded first and second derivatives in both u, and θ .

Implicitly, we are assuming functions g and p to be Lipschitz continuous on both u and θ .

Assumption 3. *Given any pair of states* $i, j \in S$, *either* $p_{ij}(u, \theta) = 0$ *for all* $u \in \mathbb{R}^K$, and $\theta \in \Theta$ or $p_{ij}(u, \theta) \ge \varepsilon > 0$, *for all* $u \in \mathbb{R}^K$, and $\theta \in \Theta$.

This is a common assumption which requires a transition to be observable for any value of the parameters (see (Borkar and Varaiya, 1979) for an example). Next, we introduce an approach to identify the unknown parameters.

A Maximum Likelihood Estimator

Let $\{i_{n-1}, i_n\}$ be a transition of the Markov chain under parameter values *u* and θ^* . A maximum likelihood estimator of θ^* given this realization is any solution to the optimization problem

$$\max_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} p_{i_{n-1}i_n}(\boldsymbol{u}, \boldsymbol{\theta}).$$

We introduce the estimating function

$$L_{i_{n-1}i_n}(u,\theta) = \frac{\partial_{\theta} p_{i_{n-1}i_n}(u,\theta)}{p_{i_{n-1}i_n}(u,\theta)} = \partial_{\theta} \log \left(p_{i_{n-1}i_n}(u,\theta) \right),$$

We note that function $L_{ij}(u, \theta)$ is simply the gradient with respect to the θ of the logarithm of the transition probability $p_{ij}(u, \theta)$. Note that since functions $p_{ij}(u, \theta)$ and $g_i(u, \theta)$ are Lipschitz continuous, and also as a consequence of Assumption 3 (see (Rudin, 1964)), it follows that the estimating function $L_{ij}(u, \theta)$ is also Lipschitz continuous. For any state $i \in S$, we define the expected direction

$$\mathscr{L}_i(u, \theta) = \sum_{j \in S} p_{ij}(u, \theta^*) L_{ij}(u, \theta).$$

Assumption 4. *The transition probabilities* $p_{ij}(u, \theta)$ *are strictly monotonic in* θ *.*

This allows us to state our first result.

Lemma 5. Under Assumption 4, we have that function $\mathscr{L}_i(u, \theta)$ is asymptotically stable around θ^* for all i, θ, u .

Proof. Suppose that $\theta \leq \theta^*$. Then, if $p_{ij}(\cdot)$ is strictly increasing (decreasing) in θ , we have that $p_{ij}(u,\theta) \leq p_{ij}(u,\theta^*)$ ($p_{ij}(u,\theta) \geq p_{ij}(u,\theta^*)$), and with derivative $\partial_{\theta}p_{ij}(u,\theta) > 0$ ($\partial_{\theta}p_{ij}(u,\theta) < 0$), and hence in all cases

$$\frac{p_{ij}(u,\theta^*)}{p_{ij}(u,\theta)}\partial_{\theta}p_{ij}(u,\theta) \geq \partial_{\theta}p_{ij}(u,\theta).$$

Therefore, using the definition of $\mathcal{L}_i(u, \theta)$, and the fact that $\sum_{j \in S} p_{ij}(u, \theta) = 1$ implies that the derivative of this sum is zero, we have

$$\mathscr{L}_{i}(u,\theta) = \sum_{j \in S} \frac{p_{ij}(u,\theta^{*})}{p_{ij}(u,\theta)} \partial_{\theta} p_{ij}(u,\theta) \ge \sum_{j \in S} \partial_{\theta} p_{ij}(u,\theta) = 0.$$

The case when $\theta^* \leq \theta$, is proved in a similar way, and yields $\mathscr{L}_i(u,\theta) \leq 0$. Finally, note that we have $\mathscr{L}_i(u,\theta) = 0$ only when $\theta = \theta^*$, which proves the result.

Recursive Estimation of Unknown Parameters

In order to estimate the value of the unknown, we rely on a simulation to sample the Markov chain. Let $\theta_0 \in \Theta$ be any initial estimate. Upon the observation of transition $i_{n-1}i_n$ of the Markov chain, under control parameters *u*, we consider the following stochastic approximation recursion

$$\boldsymbol{\theta}_{n+1} = \boldsymbol{\Pi}_{\boldsymbol{\Theta}} \left| \boldsymbol{\theta}_n + \boldsymbol{\gamma}_n \boldsymbol{L}_{i_{n-1}i_n}(\boldsymbol{u}_n, \boldsymbol{\theta}_n) \right|, \qquad (2)$$

where $\Pi_{\Theta}[\cdot]$ is a projection to the set Θ , e.g., shortest distance projection, and stepsizes γ_n satisfying the standard conditions below.

Assumption 6. The stepsizes γ_n are such that $\sum_n \gamma_n = \infty$, $\sum_n \gamma_n^2 < \infty$.

A consequence of Assumptions 4–6 is that $\theta_n \to \theta^*$ as $n \to \infty$, and it does so at the rate of $O\left(\frac{1}{\sqrt{n}}\right)$ (see for example(Ma et al., 1990)). If we define error to be $|\theta_n - \theta^*|$, we also have the following result for the sum of errors, which will be relevant for the results that follow.

Corollary 7. Under Assumptions 1-6, we have

$$\sum_n \gamma_n |\theta_n - \theta^*| < \infty.$$

Proof. Since $E[|\theta_n - \theta^*|] < \frac{C}{\sqrt{n}}$ for some constant *C*, results in $\sum_n E[\gamma_n |\theta_n - \theta^*|] < \infty$. This, and the bounded second moment

$$\sum_n \gamma_n^2 |\theta_n - \theta^*| < \infty,$$

allow us to conclude the desired result.

In the following section, we illustrate the use of this estimation procedure in optimization.

ADAPTIVE OPTIMIZATION

In this section we introduce a two time-scale that uses the estimation procedure (finer time-scale), and uses the estimates with parameter certainty to optimize the objective function by estimating the gradient of the objective. We begin this section discussing the conditions for a simulation-based procedure based on the observation of regenerative cycles. Consider any state i^* recurrent under all values of u, and consider t_0, t_1, \ldots to be the times when the chain visits this marked state. Therefore an observation $\{i_{t_m}, i_{t_m+1}, \ldots, i_{t_{m+1}}\}$ corresponds to a regenerative cycle. We state our assumptions with respect to such simulation-based optimization procedures.

Assumption 8. Suppose that given a regenerative cycle $\{i_{t_m}, i_{t_m+1}, \ldots, i_{t_{m+1}}\}$, we have a function $H(u, \theta^*; i_{t_m}, \ldots, i_{t_{m+1}})$, which for brevity we will denote $H_m(u, \theta^*)$, such that the recursion

$$u_{m+1} = u_m + \gamma_m H_m(u_m, \theta^*),$$

is such that $\lim_{m\to\infty} \nabla_u \lambda(u_m, \theta^*) = 0$, i.e., a local optima. Moreover, we assume that H is differentiable in θ , and its derivative is bounded.

To state our main result we define the following recursive procedure

$$u_{m+1} = u_m + \gamma_m H_m(u_m, \theta_{t_m}), \qquad (3)$$

during visits to state i^* , and

$$\boldsymbol{\theta}_{n+1} = \boldsymbol{\Pi}_{\boldsymbol{\Theta}} \left[\boldsymbol{\theta}_n + \boldsymbol{\mu} \, \boldsymbol{\gamma}_n \boldsymbol{L}_{i_n i_{n+1}} \left(\boldsymbol{u}_m, \boldsymbol{\theta}_n \right) \right], \tag{4}$$

during every other transition. We now state our main result.

Theorem 9. Under Assumptions 1 and 8, we have that recursive equations 3–4 are such that

$$\nabla_u \lambda(u_m, \theta^*) \to 0, \quad \theta_n \to \theta^*,$$

as $m, n \rightarrow \infty$.

Proof. To show convergence of u_m , we rewrite

$$u_{m+1} = u_m + \gamma_m H_m(u_m, \theta^*) + \varepsilon'_m,$$

where $\varepsilon'_m = \gamma_m(H(u_m, \theta_{t_m}) - H(u_m, \theta^*))$. By the mean value theorem, we can find $\hat{\theta}_m$, such that

$$\varepsilon'_{m} = \gamma_{m} \nabla_{\theta} H\left(u_{m}, \hat{\theta}_{m}\right) \left(\theta_{t_{m}} - \theta^{*}\right).$$

Then

$$\sum_{m} \|\varepsilon'_{m}\| = \sum_{m} \gamma_{m} \|H(u_{m}, \hat{\theta}_{m})(\theta_{t_{m}} - \theta^{*})\|$$

$$\leq K \sum_{m} \gamma_{m} |\theta_{t_{m}} - \theta^{*}|$$

$$< K \sum_{n} \gamma_{n} |\theta_{n} - \theta^{*}| < \infty.$$

The last inequality is a consequence of Corollary 7. Since the second moment is bounded under our assumptions, we have

$$\sum_m \varepsilon_m < \infty, \quad w.p.1.$$

The result follows from the fact that the noise introduced by the estimation procedure is asymptotically negligible.

An Instance of the Algorithm

An example of a function satisfying Theorem 9 is the (biased) gradient estimate of (Marbach and Tsitsiklis, 2001). Given a regenerative cycle $\{i_0 = i^*, i_1, \dots, i_T\}$, we consider the (biased) gradient estimate $F(u, \theta, \tilde{\lambda}) =$

$$=\sum_{n=0}^{T}\tilde{v}_{i_{n}}\left(u,\theta,\tilde{\lambda}\right)\frac{\nabla_{u}p_{i_{n-1}i_{n}}\left(u,\theta\right)}{p_{i_{n-1}i_{n}}\left(u,\theta\right)}+\nabla_{u}g_{i_{k}}\left(u,\theta\right),\quad(5)$$

where $\tilde{v}_{i_n}\left(u,\theta,\tilde{\lambda}\right) = \sum_{k=n}^{T} \left(g_{i_k}\left(u,\theta\right) - \tilde{\lambda}\right)$. It is shown in that (Marbach and Tsitsiklis, 2001) that this estimate can be used in a stochastic approximation algorithm to find a local optimum of the average reward $\lambda\left(u,\theta^*\right)$, as will be illustrated in the following section.

We introduce a simple modification to the "batch" algorithm of (Marbach and Tsitsiklis, 2001). The modified algorithm achieves the purpose of optimizing the average reward of the system, while discovering the value θ^* of the unknown parameters. The procedure starts with an initial estimate θ_0 of the unknown parameter θ^* , an initial guess of the control parameters u_0 , and an estimate $\tilde{\lambda}_0$ of $\lambda(u_0, \theta_0)$. Again, let t_m be the time of the *m*-th return to the special state i^* . At those times, new values for u_m , $\tilde{\lambda}_m$, and θ_n are calculated with the recursive formulae

$$u_{m+1} = u_m + \gamma_m F(u_m, \tilde{\lambda}_m, \theta_{t_m}), \qquad (6)$$

$$\tilde{\lambda}_{m+1} = \tilde{\lambda}_m + \eta \gamma_m \sum_{n=t_m}^{t_{m+1}-1} (g_{i_n}(u_m, \theta_{t_m}) - \tilde{\lambda}_m), \quad (7)$$

at the end of each regeneration cycle, and the recursion

$$\theta_{n+1} = \Pi_{\Theta}[\theta_n + \mu \gamma_n L_{i_n i_{n+1}}(u_m, \theta_n)], \qquad (8)$$

at every transition. Here $\eta > 0$, and $\mu > 0$ are stepsize factors. Even though the chain is different to the one being simulated (under the correct values θ^*), it will be shown that the difference is asymptotically negligible under Assumptions 1-3, in the sense that the stability of the algorithm is not compromised. Also, note that while the parameter estimate is updated during every iteration, the control parameters are only updated at the end of a regenerative cycle.

Equations 6 and 7 coincide with the "batch" algorithm introduced in (Marbach and Tsitsiklis, 2001), differing only in our use of estimates θ_{t_m} of the unknown values θ^* , and the introduction of the estimation recursion of Eqn. 8.

Convergence of the Algorithm

In this section, it will be shown that under Assumptions 1-3 the average behavior of the procedure converges asymptotically to the one with full knowledge of the parameters, and the error obtained in such process is asymptotically negligible. To set the stage for the discussion, let $r_m = (u_m, \tilde{\lambda}_m)$, and let

$$H(r_m, \theta_{t_m}) = \begin{bmatrix} F\left(u_m, \tilde{\lambda}_m, \theta_{t_m}\right) \\ \eta \sum_{n=t_m}^{t_{m+1}-1} \left(g_{i_n}(u_m, \theta_{t_m}) - \tilde{\lambda}_m\right) \end{bmatrix}, \quad (9)$$

with which the algorithm can be rewritten as:

$$r_{m+1} = r_m + \gamma_m H(r_m, \theta_{t_m}),$$

In order to apply the convergence result from the previous section, we need the following result.

Lemma 10. $H(u, \tilde{\lambda}, \theta)$ is differentiable with respect to θ , and there exists a constant C such that $E[\|\nabla H(u, \tilde{\lambda}, \theta)\|] \leq C$ for all $u, \tilde{\lambda}$, and θ .

Proof. Vector $H(u, \tilde{\lambda}, \theta)$, $F(u, \tilde{\lambda}, \theta)$, is a sum of differentiable functions $g_i(\cdot)$, $\nabla_u g_i(\cdot)$, and ratios of differentiable functions $\frac{\nabla_u p_{ij}(u, \theta)}{p_{ij}(u, \theta)}$, and therefore differentiable. Notice that the derivative of the ratio $\frac{\nabla_u p_{ij}(u, \theta)}{p_{ij}(u, \theta)}$ is bounded as a consequence that $p_{ij}(u, \theta) > \varepsilon$. A consequence of positive recurrence, is that *T* the length of a regenerative cycle satisfies $E[T] < \infty$, and $P(T > n) \le M\rho^n$, for some constant *M*. Therefore the expected value of the gradient of $H(u, \tilde{\lambda}, \theta)$ is a sum of bounded terms, which guarantees the function has bounded expectation.

This results also shows the convergence of the algorithm described by equations (6)-(8) to the true parameter value θ^* , and a local optima of the objective function.

Corollary 11. The recursive procedure described in (6)-(8) converges with probability one to $(u, \tilde{\lambda}, \theta^*)$, where $\nabla_u \lambda(u) = 0$, and $\tilde{\lambda} = \lambda(u)$, under Assumptions 1-6.

The results follows immediately from 9.

NUMERICAL ILLUSTRATION

In this section, we present a small, but illustrative example of the algorithm described in equations (6)-(8). Consider a Markov reward process with finite-state space $S = \{1, 2, ..., N\}$, with transition probabilities given by $p_{i,j}(u, \theta) =$

$$=\begin{cases} \frac{(N-i+1)u}{(N-i+1)u+\theta} & \text{if } j=i+1 \le N, \text{ or } j=i=N, \\ \frac{\theta}{(N-i+1)u+\theta} & \text{if } j=i-1>0, \text{ or } j=i=1, \text{ and} \\ 0 & \text{ otherwise,} \end{cases}$$



Figure 1: Results of Applying the Algorithm of Eqns. 6-8 (Adaptive Algorithm), Compared to the "Batch" Algorithm of (Marbach and Tsitsiklis, 2001). The Optimal Value is $u^* = .2478$



Figure 2: Evolution of the Average Reward Obtained Using the Algorithm Described in Eqns. 6-8 (Adaptive Algorithm), Compared to the "Batch" Algorithm of (Marbach and Tsitsiklis, 2001).

for $\theta \in [a,b]$, and $u \in (0,1)$. On the other hand, the reward per stage will be given by

$$g_i(u,\theta) = (1-u)\frac{(N-i+1)u}{(N-i+1)u+\theta}$$

Since both transition probabilities are monotonic in θ in all cases, for all values of *u* and *i*, Assumption 4 is satisfied, and therefore it follows that estimator $\mathcal{L}(u, \theta)$ will correctly identify the true parameter θ^* .

The results for the case N = 100, and for $u \in (0, 1)$, and $\Theta = [20, 30]$ with $\theta^* = 25$. are shown in figures 1–3. The optimal value (computed off-line) is $u^* = .2478$.

Tracking Slow Changing Parameters

To illustrate the potential of the algorithm of equations (6)–(8) for tracking, we modify it to identify slow changing conditions. Suppose that instead of a fixed but unknown parameter $\theta^* \in \Theta$, we have that $\theta^*(t), t \in \mathbb{R}^+$ is



Figure 3: Evolution of the Estimates Obtained by the Algorithm Described in Equations 6-8 Compared to the True Values



Figure 4: Algorithm of Eqns. 6-8 Using a Constant Stepsize

a function of time *t*. We first modify the algorithm mentioned above, by using a constant gain size, i.e., by using stepsizes $\gamma_t = \gamma_0$. We let $\theta^*(t)$ increase linearly from 20 to 30 during the first half of the experiment, and then, we let it drop down linearly to 20 for the other half of the experiment. The results are shown in figures (4)–(5b).

CONCLUSIONS

We have presented a two-time-step approach that uses simulation to identify unknown system parameters and select optimal parameters for controllable Markov chains. These approach results in a family of algorithms that are robust to parametric uncertainty, in that they 1) compute estimates of unknown but fixed parameters, and 2) maximize the average reward by moving the tunable parameters in the gradient of the objective function, estimated through simulation via parameter certainty. We provide sufficient conditions for the convergence of such algorithm, and illustrate an instance of it through the application of the identification algorithm to an existing gradient estimate. As was shown here through a small numerical example, using a constant stepsize produces



(a) Evolution of the Average Reward Obtained Using the Algorithm described in Eqns. 6-8 and Using a Constant Stepsize.



(b) Evolution of the Estimates Obtained by the Algorithm Described in Equations 6-8 with a Constant Stepsize

an algorithm with the ability to track slowly changing parameters. In (Campos-Nanez and Patek, 2003), a similar approach is used to address the larger problem of realtime pricing/revenue management in networks.

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ADAPTIVE CONTROL OF THE TUBULAR REACTOR WITH CO- AND COUNTER-CURRENT COOLING IN THE JACKET

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ABSTRACT

This paper deals with the adaptive control of the tubular chemical reactor as a typical member of nonlinear system with continuously distributed parameters. Although this system has negative control properties, proposed adaptive controller which uses external linear model and recursive identification provides good control results. This controller is designed with the use of polynomial approach which satisfies basic control requirements. The main benefit of the counter-current cooling compared with co the co-current can be found in the cooling effectiveness which is better from the control point of view too. The controller could be tuned via position of the closed-loop root.

INTRODUCTION

The role and usage of the simulation increases every day with the rapidly growing computer power and slumping costs of today's computers. Mathematical description is in this case very important and helps us with the constructing of the so called mathematical model (Luyben 1989). The computer simulation of systems described by the mathematical model then usually consist of static and dynamic analyses which describe the behaviour of the system in the steady-state and after the step change of the input variable. These analyses usually results in the optimal working point where the production is the highest or the costs are the lowest.

Tubular chemical reactor is tool frequently used in chemical industry for production of the several chemicals. This type of reactor belongs to the class of systems with distributed parameters because state variables here depend not only on the time variable but on the space variable too (Ingham *et al.* 2000). Configuration with one main pipe with several pipes inside used in this work offers cooling in the remaining space of the main pipe with the same or opposite direction to the flow direction of the reactant. This is in this paper called co- and counter-current cooling.

Controlling of such processes with conventional methods such as Ziegler-Nichols etc. could be problem

mainly in the cases where the working point changes. This inconvenience should be overcome with the use of some of "new" control strategies such as adaptive control, predictive control etc. This work show process of the designing of the adaptive controller (Bobál *et al.* 2005). The adaptation is process known from the animals and plants which adapts their behaviour to the environment. This process means the loss of the energy collects information and experiences about the system.

Adaptive approach here is based on the choice of the External Linear Model (ELM) of originally nonlinear system, parameters of which are estimate recursively and parameters of the controller are recomputed in each step according these identified ones.

The delta models (Mukhopadhyay *et al.* 1992) were used in ELM. Although these models belongs to the class of discrete-time models, parameters of such models approaches to the continuous-time ones for small sampling period (Stericker and Sinha 1993).

The polynomial approach together with the poleplacement method (Kučera 1993) which are used for the designing of the controller satisfy basic control requirements such as stability, disturbance attenuation or reference signal tracking.

All simulations were done in the mathematical simulation software Matlab, version 6.5.

MATHEMATICAL MODEL OF THE PLANT

As it is written above, this work compares two types of tubular chemical reactors varying in the direction of the cooling in the jacket.

The mathematical model of this system comes from material and heat balances inside the reactor. We consider ideal plug-flow tubular chemical reaction with a simple exothermic consecutive reaction $A \rightarrow B \rightarrow C$ in the liquid phase (Dostál *et al.* 1996). Mathematical description of such process is very complex and so we introduce some simplifications. We neglect heat losses and conduction along the metal wall of the pipes, but heat transfer through the wall is consequential for a dynamic study. Furthermore, we expect that all densities, heat capacities and heat transfer coefficients are constant.

The graphical representation of the tubular chemical reactor can be found in Figure 1.



Figure 2: Tubular chemical reactor with co- (solid line) and counter-current (dashed line) cooling in the jacket

The mathematical model is in this case described by the set of five PDE derived from the balances inside the reactor:

$$\frac{\partial c_A}{\partial t} + v_r \cdot \frac{\partial c_A}{\partial z} = -k_1 \cdot c_A \tag{1}$$

$$\frac{\partial c_B}{\partial t} + v_r \cdot \frac{\partial c_B}{\partial z} = k_1 \cdot c_A - k_2 \cdot c_B$$
(2)

$$\frac{\partial T_r}{\partial t} + v_r \cdot \frac{\partial T_r}{\partial z} = \frac{Q_r}{\rho_r \cdot c_{rp}} - \frac{4 \cdot U}{d_1 \cdot \rho_r \cdot c_{pr}} \cdot (T_r - T_w)$$
(3)

$$\frac{\partial T_{w}}{\partial t} = \frac{4 \cdot \left[d_{1} U_{1} (T_{r} - T_{w}) + d_{2} U_{2} (T_{c} - T_{w}) \right]}{\left(d_{2}^{2} + d_{1}^{2} \right) \cdot \rho_{w} \cdot c_{pw}}$$
(4)

These four PDE are common for both co- and countercurrent cooling. The difference can be found in the last PDE which comes from the heat balance of the cooling liquid.

This equation has for co-current cooling form:

$$\frac{\partial T_c}{\partial t} + v_c \cdot \frac{\partial T_c}{\partial z} = \frac{4 \cdot n_1 \cdot d_2 \cdot U_2 \cdot (T_w - T_c)}{\left(d_3^2 - n_1 \cdot d_2^2\right) \cdot \rho_c \cdot c_{pc}}$$
(5)

and for counter-current cooling:

$$\frac{\partial T_c}{\partial t} - v_c \cdot \frac{\partial T_c}{\partial z} = \frac{4 \cdot n_1 \cdot d_2 \cdot U_2 \cdot (T_w - T_c)}{\left(d_3^2 - n_1 \cdot d_2^2\right) \cdot \rho_c \cdot c_{pc}}$$
(6)

where *T* is the temperature, *d* represents diameters, ρ are densities, c_p means specific heat capacities, *U* stands for the heat transfer coefficients, n_1 is a number of tubes and *L* represents the length of the reactor. Index $(\bullet)_r$ means the reaction compound, $(\bullet)_w$ is for the metal wall of the pipes and $(\bullet)_c$ for the cooling liquid. Variables v_r and v_c are fluid velocities of the reactant and cooling liquid, respectively, as

$$v_r = \frac{q_r}{f_r}; \quad v_c = \frac{q_c}{f_c} \tag{7}$$

where q are flow rates and f are constants

$$f_r = n_1 \cdot \frac{\pi \cdot d_1^2}{4}; \quad f_c = \frac{\pi}{4} \cdot \left(d_3^2 - n_1 \cdot d_2^2 \right)$$
 (8)

The reaction velocities, k_i , in equations (1) - (2) and equations are nonlinear functions of the temperature computed via the Arrhenius law:

$$k_j = k_{0j} \cdot \exp \frac{-E_j}{R \cdot T_r}, \text{ for } j = 1,2$$
(9)

where k_{0j} represents pre-exponential factors, *E* means activation energies and *R* is a gas constant. Q_r in the equation (3) is reaction heat computed as

$$Q_r = h_1 \cdot k_1 \cdot c_A + h_2 \cdot k_2 \cdot c_B \tag{10}$$

and h_j is used for reaction enthalpies.

The mathematical model shows that this plant is a nonlinear system with continuously distributed parameters (Ingham et al. 2000). Strong nonlinearity can be found in Equation (3), and the system is with distributed parameters because of the presence of the PDE where the state variable is related not only to the time variable, t, but the space variable, z, too.

In this case the initial conditions are $c_A(z,0) = c_A^{s}(z)$, $c_B(z,0) = c_B^{s}(z)$, $T_r(z,0) = T_r^{s}(z)$, $T_w(z,0) = T_w^{s}(z)$ and $T_c(z,0) = T_c^{s}(z)$ and boundary conditions $c_A(0,t) = c_{A0}(t)$, $c_B(0,t) = c_{B0}(t) = 0$, $T_r(0,t) = T_{r0}(t)$, $T_c(0,t) = T_{c0}(t)$ for the *co-current* cooling and $T_c(L,t) = T_{cL}(t)$ for the *countercurrent* cooling.

Fixed parameters of the reactor (Dostál *et al.* 1996) are shown in the following table:

Table 1: Fixed parameters of the tubular reactor

$d_1 = 0.02 m$	$c_{pc} = 4.18 \ kJ.kg^{-1}.K^{-1}$
$d_2 = 0.024 m$	$U_1 = 2.8 \ kJ.m^{-2}.K^{-1}.s^{-1}$
$d_3 = 1 m$	$U_2 = 2.56 \ kJ.m^{-2}.K^{-1}.s^{-1}$
$n_1 = 1200$	$k_{10} = 5.61 \times 10^{16} s^{-1}$
L = 6 m	$k_{20} = 1.128 \times 10^{16} s^{-1}$
$q_r = 0.15 \ m^3 . s^{-1}$	$E_1/R = 13477 \ K$
$q_c = 0.275 \ m^3 . s^{-1}$	$E_2/R = 15290 K$
$\rho_r = 985 \ kg.m^3$	$h_1 = 5.8 \times 10^4 \ kJ.kmol^{-1}$
$\rho_w = 7800 \ kg.m^3$	$h_2 = 1.8 \times 10^4 \ kJ.kmol^{-1}$
$\rho_c = 998 \ kg.m^3$	$c_{A0}^{s} = 2.85 \ kmol.m^{-3}$
$c_{pr} = 4.05 \ kJ.kg^{-1}.K^{-1}$	$T_{r0}^{s} = 323 K$
$c_{pw} = 0.71 \ kJ.kg^{-1}.K^{-1}$	$T_{c0}^{s} = 293 K$

STEADY-STATE AND DYNAMIC ANALYSES

The steady-state and dynamic analyses are important parts in the design of the controller especially in the simulation cases. Results of these analyses gives us overview of the system's static and dynamic behaviour. From the mathematical point of view, the static analysis means solving of the set of PDE (1) - (6) for the time $t \rightarrow \infty$, which means that all derivatives with respect to time are equal to zero. But there are still derivatives with respect to axial variable.

These derivatives can be replaced from the mathematical point of view by the first back (co-current cooling) and forward (counter-current cooling) differences :

$$\frac{dx}{dz}\Big|_{z=z_i} \approx \frac{x(i) - x(i-1)}{h_z}, \text{ for } i = 1, 2, \dots, n$$

$$\frac{dx}{dz}\Big|_{z=z_j} \approx \frac{x(j+1) - x(j)}{h_z}, \text{ for } j = n, n-1, \dots, 0$$
(11)

where x is a general variable, h_z is an optional size of the step in axial direction. The defined input boundary conditions, x_0 , for i = 1 are equal to boundary conditions x(0). If the reactor is divided into N_z equivalent parts, the discretization step is

$$h_z = \frac{L}{N_z} \tag{12}$$

where *L* denotes the length of the reactor and $N_z = 100$. The steady-state analysis was performed for the different volumetric flow rate of the cooling $q_c^s = <0.1$; $0.35 > [m^3.s^{-1}]$ in the jacket and the results for both coand counter-current cooling are shown in Figure 3 and Figure 4. It can be clearly seen that counter-current cooling results in high nonlinearity whereas in cocurrent cooling the variables are close to linear course.



Figure 3: Steady-state analysis of the temperature of the reactant T_r^s for co-current cooling



Figure 4: Steady-state analysis of the temperature of the reactant T_r^s for counter-current cooling

The steady-state analysis results in the working point which is in this case defined by the volumetric flow rate of the reactant $q_r^s = 0.150 \ m^3.s^{-1}$ and the volumetric flow rate of the coolant $q_c^s = 0.275 \ m^3.s^{-1}$. These variables are later used for dynamic analysis and simulation of the control.

The dynamic analysis is the next step after the steadystate analysis. It examines the behaviour after the step change of one of the input variables. Because the set of PDE (1) - (6) has derivatives with the respect to axial variable z, the discretization described by equations (11) must be used. The set of PDE is then transformed to a set of ODE which is then solved by the standard Runge-Kutta's method.

This analysis was done for four step changes $\pm 20\%$ and $\pm 10\%$ of the volumetric flow rate of the cooling liquid, Δq_c^s , i.e. -0.055 (-20%), -0.0275 (-10%), 0.0275 (10%), 0.055 (20%) $m^3.s^{-1}$. The output variable y(t) illustrate the difference between the actual values of the reactive temperature, T_r , at the end of the reactor (z = L) and its steady-state value T_r^s . These input and output variables should be mathematically described as

$$u(t) = \frac{q_c(t) - q_c^s}{q_c^s} \cdot 100[\%]$$

$$y(t) = T_r(t, L) - T_r^s(L)[K]$$
(13)



Figure 5: Output responses for various step changes Δq_c^s and co-current cooling



Figure 6: Output responses for various step changes $\Delta q_c^{\ s}$ and counter-current cooling

The output responses for both cooling techniques displayed in Figure 5 and Figure 6 shows that this output should be expressed by second order transfer function with relative order one for the case of non-minimum phase behaviour:

$$G(s) = \frac{b(s)}{a(s)} = \frac{b_1 s + b_0}{s^2 + a_1 s + a_0}$$
(14)

The last graphs in Figure 7 and Figure 8 compares dynamic behaviour for co- and counter-current cooling. The result is obvious – cooling capability of the counter-current cooling is at least twice bigger than for the co-current cooling with the same input step change. This feature was proofed and developed in deep detail in (Vojtěšek *et al.* 2006).



Figure 7: Comparison of co-current and countercurrent cooling for step change $\Delta q_c^s = -20\%$



Figure 8: Comparison of co-current and countercurrent cooling for step change $\Delta q_c^s = +20\%$

ADAPTIVE CONTROL

As it is written above, results from the dynamic analysis helps with the choice of the External Linear Model (ELM) (14). The adaptive approach here is based on the recursive parameter identification of the ELM and parameters of the controller are recomputed according to the estimated parameters in every step too (Bobál *et al.* 2005).

The adaptive controller is designed via polynomial synthesis (Kučera 1993) which fulfills basic control requirements and it can be used for systems with negative control properties.

The basic control configuration with one degree-offreedom displayed in Figure 9 was used.



Figure 9: One degree-of-freedom control configuration

Block Q in Figure 9 represents the transfer function of the controller, G denotes the transfer function of the plant, w is the reference signal, e is used for the control error, v is the disturbance at the input to the system, u determines the input variable, and finally y is the output variable. Polynomials a(s) and b(s) in the transfer function (14) are commensurable polynomials in complex *s*-plane. The realizability condition is fulfilled if the system is proper, i.e. deg $a(s) \ge deg b(s)$. The transfer function of the controller then is

 $\tilde{Q}(s) = \frac{q(s)}{s \cdot \tilde{p}(s)}$ (15)

where polynomials q(s) and $\tilde{p}(s)$ are computed from the Diophantine equation

$$a(s) \cdot s \cdot \tilde{p}(s) + b(s) \cdot q(s) = d(s)$$
(16)

by the method of uncertain coefficients which compares coefficients of individual *s*-powers. The polynomial d(s) on the right side of (16) is stable optional polynomial which fulfills the stability of the controller.

Degrees of the polynomials q(s), $\tilde{p}(s)$ and d(s) are for the transfer function (14)

$$\deg \tilde{p}(s) \ge \deg a(s) - 1 = 1 \deg q(s) = \deg a(s) = 2 \deg d(s) = \deg a(s) + \deg \tilde{p}(s) + 1 = 4$$

$$(17)$$

which means that the transfer function of the controller in Equation (15) could be rewritten to form

$$\tilde{Q}(s) = \frac{q(s)}{s \cdot \tilde{p}(s)} = \frac{q_2 s^2 + q_1 s + q_0}{s \cdot (p_1 s + p_0)}$$
(18)

The optional polynomial d(s) is in our case

$$d(s) = m(s) \cdot n(s) \tag{19}$$

where m(s) is $m(s)=(s+\alpha)^2$ for $\alpha>0$ and n(s) comes from the spectral factorization of a(s):

$$n^{*}(s) \cdot n(s) = a^{*}(s) \cdot a(s) \Rightarrow \frac{n_{0} = \sqrt{a_{0}^{2}}}{n_{1} = \sqrt{a_{1}^{2} + 2n_{0} - 2a_{0}}}$$
(20)

Polynomials a(s) and b(s) in (14) and (18) are known from the recursive identification.

The delta models were used for the estimation model. Although the delta models belong to the class of discrete-time models, parameters of such model approach to the continuous-time model for small sampling period (Stericker and Sinha 1993).

The transfer function G(s) in (14) could be rewritten to the form of differential equation:

$$y_{\delta}(k) = -a'_{1}y_{\delta}(k-1) - a'_{0}y_{\delta}(k-2) + +b'_{1}u_{\delta}(k-1) + b'_{0}u_{\delta}(k-2)$$
(21)

which is in the vector form

$$y_{\delta} = \boldsymbol{\theta}_{\delta}^{T}(k) \cdot \boldsymbol{\phi}_{\delta}(k-1)$$
(22)

and the vector of the parameters, θ_{δ} , and the data vector, φ_{δ} , are then

$$\boldsymbol{\theta}_{\boldsymbol{\delta}}(k) = \left[a'_{1,}a'_{0,}b'_{1,}b'_{0}\right]^{T}$$
$$\boldsymbol{\phi}_{\boldsymbol{\delta}}(k-1) = \left[-y_{\boldsymbol{\delta}}(k-1), -y_{\boldsymbol{\delta}}(k-2), \dots \right]^{T}$$
$$(23)$$
$$\dots, u_{\boldsymbol{\delta}}(k-1), u_{\boldsymbol{\delta}}(k-2)\right]^{T}$$

$$y_{\delta}(k) = \frac{y(k) - 2y(k-1) + y(k-2)}{T_{\nu}^{2}};$$

$$y_{\delta}(k-1) = \frac{y(k-1) - y(k-2)}{T_{\nu}}; \quad y_{\delta}(k-2) = y(k-2) \quad (24)$$

$$u_{\delta}(k-1) = \frac{u(k-1) - u(k-2)}{T_{\nu}}; \quad u_{\delta}(k-2) = u(k-2)$$

The goal of the identification is to estimate vector of parameters θ_{δ} in ARX model (22) from the previous values of the input and output variables in the time intervals remote by sampling period $T_{\underline{\nu}}$. The recursive least-squares method with exponential forgetting was used for identification in this work (Fikar and Mikleš 1999).

SIMULATION RESULTS

The input and output variables, initial values and settings in the simulation experiments are the same as in the dynamic analysis described by the Equation (13). The simulation time is $T_f = 10\ 000$ seconds and 5 different step changes were done during this time.

The sampling time for counter-current cooling was $T_v = 1.5 \ s$ and simulations were done for three values of the parameter $\alpha = 0.007, 0.01$ and 0.02. The results are shown in Figure 10 and 11.



Figure 10: The course of the output variable y(t) for different parameter α for counter-current cooling



Figure 11: The course of the input variable u(t) for different parameter α for counter-current cooling

It can easily seen from the figures that increasing value of parameter α results mainly in quicker output response. On the other hand, low value of α produces smoother course of the input variable u(t) which is better from the practical point of view. The input variable is in our case represented by the volumetric flow rate of the coolant which could be reduced by the valve and shocking twists of the valve could demage or destroy it.



Figure 12: The course of the output variable y(t) for different parameter α for co-current cooling



Figure 13: The course of the input variable u(t) for different parameter α for co-current cooling



Figure 14: Comparison of the output response of the coand counter- current cooling for $\alpha = 0.01$

The control analysis for co-current cooling was performed for the same settings as for counter-current cooling for the reason of comparability but the results for sampling period were unacceptable and it was decreased to its half value, i.e. $T_v = 0.75 \ s$. The results presented in Figure 12 and 13 shows the same effect of the value as for counter-current cooling.

Figures 14, 15, 16 and 17 clearly shows the main benefits of the counter-current cooling. This type of cooling has better effectiveness which reflects mainly in the course of the input variable u(t) which is smoother and its value is lower than for co-current cooling. The output variable y(t) has smoother and quicker course too.



Figure 15: The course of the input variable for the coand counter- current cooling, $\alpha = 0.01$



Figure 16: Comparison of the output response of the coand counter- current cooling for $\alpha = 0.02$

Because we wanted to have some mathematical tool to compare obtained results, the control quality criteria S_u and S_y were introduced:

$$S_{u} = \sum_{i=2}^{N} (u(i) - u(i-1))^{2} [-]; \quad \text{for } N = \frac{T_{f}}{T_{v}}$$

$$S_{y} = \sum_{i=1}^{N} (w(i) - y(i))^{2} [K^{2}];$$
(25)

Values of these criterions clearly shows benefits of the counter-current cooling in the jacket which are lower than for co-current cooling in more cases. The values for both types of cooling are displayed in Table 2 and highlighted in Figures 18 and 19.



Figure 17: The course of the input variable for the coand counter- current cooling, $\alpha = 0.02$

Table 2: Control quality criteria S_u and S_v

	Co-current cooling		Counter-current cooling	
	<i>S</i> _{<i>u</i>} [-]	S_{y} [-]	S_u [-]	<i>S</i> _y [-]
$\alpha_1 = 0.007$	320 680.51	2 179.02	31 779.06	3 029.87
$\alpha_1 = 0.01$	11 916.77	5 077.97	31 107.32	1 922.40
$\alpha_1 = 0.02$	38 361.72	1 975.38	10 522.22	1 161.74



Figure 18: Values of the control quality criterion S_u for co- and counter-current cooling



Figure 19: Values of the control quality criterion *S_y* for co- and counter-current cooling

CONCLUSIONS

The goal of this contribution was mainly to show simulation results of the adaptive control used for the controlling of the reactant's temperature via volumetric flow rate of the coolant in the jacket. Used adaptive approach which estimates parameters of the ELM produces good control results although the system has negative control properties such as nonlinearity, time delay etc. The controller could be tuned by the choice of the parameter α which is position of the root. The increasing value of α results in quicker output response but bigger overshoots. The comparison of co-current and counter-current cooling in the jacket clearly shows that cooling with opposite direction to the flow of the reactant has better effectiveness than cooling which flows with the same direction as the reactant. Another advantage could be found in sampling period which is twice bigger for the counter-current cooling than for cocurrent with comparably good results.

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DESCRIPTION AND ANALYSIS OF INTERVAL SYSTEMS

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KEYWORDS

Interval Uncertainty, Robust Stability, Kharitonov Theorem, Value Set Concept, Zero Exclusion Condition.

ABSTRACT

Control of real industrial processes is almost always burden with an uncertainty. The reasons of that unfavorable fact are mainly an imprecise modelling and measuring or an influence of some external conditions. A convenient tool for dealing with such class of issues represents the application of models with parametric uncertainty. The mathematical model is then supposed to contain parameters which are not precisely known, but the values thereof lie within given intervals. If individual uncertain coefficients (in polynomial, in transfer function etc.) are mutually independent, the uncertainty has a simple interval structure. This contribution offers several possibilities of utilization of interval uncertainty for systems description and presents the tools for robust stability analysis, emphasizing advantages and limitations connected with the use of this simple structure, even for more complicated problems.

INTRODUCTION

During the second half of the last century, the one of thorny problems emerged in theory of automatic control. New analytical methods of synthesis, which assume an exact mathematical model of the process to be controlled, paid insufficient attention to uncertainty caused by imperfections in modelling or changeable physical properties of the plant. On that account, uncertain systems have become very attractive from the point of view of scientific research and also applications during previous almost three decades. It is fully natural, that number of approaches that solve the related problems has been developed and improved during this long-term interest.

The classical and probably also the most required task is to ensure appropriate control of the system which is affected by some changes, variations, perturbations or disturbances. Generally, more basic principles how to solve these issues exist. A relatively clear and comprehensible idea is incorporated in robust control. Its aim is to design the one fixed controller which guarantees suitable behaviour not only for nominal system, but also for some neighbourhood. Robust controllers are preferred in contemporary practice, simple and easily utilizable. On the contrary, the abilities of these compensators are limited at great or fast changes in controlled system or operating conditions and, furthermore, robust control responses need not to "optimal" for all supposed states.

This contribution is focused mainly on problems of description and analysis of systems with interval uncertainty and their importance in theory and practice of process control. Interval uncertainty and related tools for robust stability testing represent essentials which many authors draw upon it during the research of analysis and synthesis methods for more complicated parametric uncertainties and moreover, the theory is also quite well applicable for practical robust control problems. First, the paper outlines the motivation for use of uncertain mathematical model and provides the categorization of basic robustness terms. Further, it is shown a possible notation of interval polynomials and several tools for analytical and graphical testing of robust stability (such as Kharitonov theorem, the value set concept and the zero exclusion condition) are presented. Finally, the possible utilization of the interval uncertainty theory for more complicated uncertainty structures is discussed.

MATHEMATICAL MODEL WITH UNCERTAINTY

Most of the technological processes can be modelled as linear time-invariant systems, in spite of the fact, that their real behaviour is often different and much more complex. The motivation is evident - owing to this, the transfer functions can be used for description of such systems and subsequently also the control theory of linear systems, which is very well-developed, can be applied. However, an effort to create the simple enough model almost always leads to the origin of uncertainty. Their emergence often consists in neglect of "less important properties", especially from the realms of fast dynamic effects, nonlinearities or time-variant behaviours of the plant.

Nevertheless, the presence of uncertainty can not be excluded even if the processes are in essence linear, because, strictly speaking, the physical parameters are never exactly known, possibly they can vary according to operating conditions. Ergo the principal problem is, if the controller designed for nominal system is able to keep some properties of the feedback control loop also for really controlled system, which falls into certain

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) neighbourhood. In other words, if the controller can keep these properties not only for one nominal system, but for the whole family of systems (Kučera 2001).

The uncertainty in constructed mathematical model and thus the size of neigbourhood which should the controller cope with can be taken into consideration and described in the two main ways – as parametric or nonparametric uncertainty. The former, nonparametric description of uncertainty lies in restriction of area of possible appearance of frequency characteristic. It is associated with unmodelled dynamics, truncation of high frequency modes, nonlinearities, randomness in the systems, etc. The latter, parametric approach then represents known structure but uncertain knowledge of actual physical parameters of the controlled system. Their possible values are usually bounded by intervals. This work deals mainly with interval systems, that is one class of systems with parametric uncertainty.

The systems with parametric uncertainty are often described via a vector of real uncertain parameters q. In a simplified way, vector q is called the uncertainty.

The very frequent subject of investigation is the uncertain characteristic polynomial of the closed-loop control system. Assume that this polynomial is described by:

$$p(s,q) = \sum_{i=0}^{n} \rho_i(q) s^i \tag{1}$$

where ρ_i are coefficient functions.

In robustness problems, the vector of uncertain parameters q is usually supposed to be confined by the uncertainty bounding set Q, which is given a priory (from identification, by user requirements, etc.). The set Q is taken to be a ball in some appropriate norm. Combination of the polynomial (1) with its uncertainty bounding set Q constitutes a family of polynomials.

The robustness issues consist in several tasks. The problem investigated in this contribution is robust stability analysis. Generally, suppose that every member of family F (family of polynomials) has a property S (stability) – the family F is then designated as robust (robustly stable).

It is well-known that the continuous-time polynomial p(s) is stable if and only if all its roots lie in the left half of the complex plane or, in other words, if and only if all its roots have negative real part. The general family of polynomials $P = \{p(\cdot,q) : q \in Q\}$ is robustly stable if and only if $p(\cdot,q)$ is stable for all $q \in Q$, i.e. all roots of p(s,q) must be located in the left complex half plane for all $q \in Q$.

The uncertainty enters into the polynomial (1) through the coefficient functions $\rho_i(q)$. And the way how the uncertain parameters enter into the coefficients of this polynomial is very significant. In accordance with this, several basic structures of uncertainty with increasing generality are distinguished:

independent (interval) uncertainty structure

- affine linear uncertainty structure
- multilinear uncertainty structure
- nonlinear uncertainty structure (polynomial, general)

Moreover, the single parameter uncertainty is considered as a special case.

This paper deals deeply only with the case of Q in the shape of box (which corresponds L_{∞} norm) and independent uncertainty structure.

INTERVAL UNCERTAINTY

The basic case of an uncertainty structure is the interval uncertainty. The essential condition is the independence of its structure. An uncertain polynomial (1) is said to have an independent uncertainty structure if each component q_i of q enters into only one coefficient. A family of polynomials:

$$P = \left\{ p(\cdot, q) : q \in Q \right\}$$
(2)

is called an interval polynomial family (or an interval polynomial for short) if it has an independent uncertainty structure, each coefficient depends continuously on q and Q is a box. The examples are:

$$p_{1}(s,q) = (3+q_{1})s^{2} + (5+q_{2})s + (2+q_{3})$$

$$q_{1} \in \langle 0.5; 2 \rangle, q_{2} \in \langle -1; 3 \rangle, q_{3} \in \langle 1; 2 \rangle$$
(3)

$$p_{2}(s,q) = s^{2} + (8 + 3q_{1} + 2q_{2})s + (5 + 2q_{3} - q_{4})$$

$$q_{i}| \leq 1$$
(4)

Such a representation of the interval uncertainty relatively often involves a redundancy – see the second polynomial (4). Therefore, simplified notation in which each uncertain coefficient is expressed only as an interval is used instead. The new family is sometimes called a lumped version of the original one. For example, the uncertainty incorporated in (4) can be easily "lumped" by defining of new uncertain parameters:

with respective new uncertainty bounding set:

$$\tilde{q}_1 \in \langle 3; 13 \rangle; \quad \tilde{q}_0 \in \langle 2; 8 \rangle$$
(6)

and the new uncertain polynomial:

$$\tilde{p}(s,\tilde{q}) = s^2 + \tilde{q}_1 s + \tilde{q}_0 \tag{7}$$

Naturally, the resulting polynomial is shortly written as:

$$\tilde{p}(s,\tilde{q}) = s^2 + [3;13]s + [2;8]$$
(8)

Generally speaking, the ordinarily used shorthand notation of an interval polynomial looks like:

$$p(s,q) = \sum_{i=0}^{n} \left[q_i^{-}; q_i^{+} \right] s^i$$
(9)
THE KHARITONOV THEOREM

The veritable milestone in robust stability analysis of systems under parametric uncertainty has become the Kharitonov theorem (Kharitonov 1979). Even though it was published in a Russian differential equations journal as early as in 1978, it has been "discovered" for the control community by Barmish (Barmish 1983; Barmish 1994) and also Bialas (Bialas 1983) entire four years later. This fundamental theorem says that an interval polynomial family with invariant degree is stable if and only if its four Kharitonov polynomials are stable. Thus, it is not necessary to check the stability of all possible extreme variations (which is 2^{l} if $q \in \mathbf{R}^{l}$), but always only of four polynomials without regard to the number of uncertain parameters. It is obvious that this reduction is of immense significance. The construction of Kharitonov polynomials is very simple and based on special fixed sequence of upper and lower bounds of coefficients in interval polynomial (9) according to the scheme:

$$K_{1}(s) = q_{0}^{-} + q_{1}^{-}s + q_{2}^{+}s^{2} + q_{3}^{+}s^{3} + \cdots$$

$$K_{2}(s) = q_{0}^{+} + q_{1}^{+}s + q_{2}^{-}s^{2} + q_{3}^{-}s^{3} + \cdots$$

$$K_{3}(s) = q_{0}^{+} + q_{1}^{-}s + q_{2}^{-}s^{2} + q_{3}^{+}s^{3} + \cdots$$

$$K_{4}(s) = q_{0}^{-} + q_{1}^{+}s + q_{2}^{+}s^{2} + q_{3}^{-}s^{3} + \cdots$$
(10)

. .

The application of Kharitonov theorem illustrates the next example. The task is to decide on the stability of the interval polynomial:

$$p(s,q) = [0.5; 1.5]s^{3} + [3; 4]s^{2} + [1; 2]s + [0.5; 1] \quad (11)$$

All four Kharitonov polynomials:

$$K_{1}(s) = 0.5 + 1s + 4s^{2} + 1.5s^{3}$$

$$K_{2}(s) = 1 + 2s + 3s^{2} + 0.5s^{3}$$

$$K_{3}(s) = 1 + 1s + 3s^{2} + 1.5s^{3}$$

$$K_{4}(s) = 0.5 + 2s + 4s^{2} + 0.5s^{3}$$
(12)

are stable and hence the original interval polynomial (11) is also stable.

An advantageous software environment for robust stability analyis of systems with parametric uncertainty represents Polynomial Toolbox for Matlab (Polyx 2009; Šebek et al. 2000). The Kharitonov polynomials can be constructed in the Polynomial Toolbox via the command "kharit".

The original Kharitonov's proof of his theorem is complicated and relatively hard to understand. Substantially simpler geometric proofs can be found e.g. in (Anagnost et al. 1989; Dasgupta 1988; Minnichelli et al. 1989) or in (Matušů and Prokop 2008).

Besides, an array of improvements of the Kharitonov theorem can be found in literature. Among the most frequent ones the following are counted: the simplification for low-degree polynomials (e.g. for the polynomial degree n = 3 and $q_0^- > 0$ to check K_3 is enough) (Anderson et al. 1987); extensions with degree dropping (Barmish 1994); an alternative technique of robust stability investigation in a form of positivity condition of the frequency sweeping function (Barmish 1989); or Kharitonov's generalization of his theorem for an interval polynomials with complex coefficients (Barmish 1994; Kharitonov 1979).

KHARITONOV RECTANGLES

The Kharitonov rectangles are special kind of the value set, which will be generally defined later and which plays the essential role in solving robust stability problems. Suppose an interval polynomial (9) and substitute the complex variable *s* for $j\omega$ with a fixed real frequency ω_0 . The value set of interval polynomial is then a two-dimensional set of all possible complex values which arise in complex plane letting *q* range over the *Q*, i.e. letting all coefficients range over their intervals. Such a value set is always of a rectangular shape (rarely line segment as a special degraded case) and its sides are parallel to the axis. As mentioned above, this value set is called Kharitonov rectangle for the frequency ω_0 .

The fig. 1 shows the Kharitonov rectangle of interval polynomial (11) for frequency $\omega_0 = 0.2$ with highlighted vertexes.



Figure 1: Kharitonov rectangle of interval polynomial (11) for $\omega_0 = 0.2$

Increasing of ω results in motion of the Kharitonov rectangle, i.e. a rectangle moves around the complex plane – see fig. 2, where Kharitonov rectangles for interval polynomial (11) are depicted (with the assistance of the Polynomial Toolbox command "khplot") for frequencies $\omega \in \langle 0, 1 \rangle$ in the range of 50 samples.



Figure 2: Kharitonov rectangles of interval polynomial (11) for $\omega \in \langle 0; 1 \rangle$

GRAPHICAL TEST OF ROBUST STABILITY

An interval polynomial family $P = \{p(s,q) : q \in Q\}$ with invariant degree and at least one stable member $p(s,q^0)$ is robustly stable if and only if the Kharitonov rectangles are excluded from the origin of the complex plane at all nonnegative frequencies, that is $0 \notin p(j\omega,Q) \quad \forall \omega \ge 0$. This rule, known as the zero exclusion condition, is very important, because in conjunction with the value set concept it represents powerful and sometimes practically the one and only conceivable method of robust stability analysis for much more complicated uncertainty structures (the coefficients must be continuous functions on given intervals). The usage of this test is essentially superfluous in the case of interval uncertainty, because the Kharitonov theorem is simpler, nevertheless the main ideas can be easily graphically verified and demonstrated – see e.g. fig. 2, where the interval polynomial family (11) contains a stable member and the zero point is excluded from the Kharitonov rectangles and hence the family is robustly stable. If the rectangles encompass the origin, it is apparent that the family will harbour the polynomial with root on imaginary axis (the stability border) - remember also the classical stability testing of polynomials via the Mikhailov(-Leonhard) criterion (Mikhailov 1938). The example of robustly unstable interval polynomial can be:

$$p(s,q) = s^{5} + [3;5]s^{4} + [5.5;10]s^{3} + [6.5;10]s^{2} + + [3;5]s + [0.5;1]$$
(13)

The Kharitonov rectangles, plotted again in the Polynomial Toolbox (for frequencies $\omega \in \langle 0; 3 \rangle$ with the step 0.015), for this once cross the zero as shown in fig. 3 and fig. 4, while the second graph is zoomed to see better what is happening in the neighbourhood of the point [0; 0*i*]. Therefore, the interval polynomial (13) is not robustly stable. In addition, it can be readily

confirmed by the stability of only three of four Kharitonov polynomials – the unstable one is $K_2(s)$.

$$K_{1}(s) = 0.5 + 3s + 10s^{2} + 10s^{3} + 3s^{4} + s^{5}$$

$$K_{2}(s) = 1 + 5s + 6.5s^{2} + 5.5s^{3} + 5s^{4} + s^{5}$$

$$K_{3}(s) = 1 + 3s + 6.5s^{2} + 10s^{3} + 5s^{4} + s^{5}$$

$$K_{4}(s) = 0.5 + 5s + 10s^{2} + 5.5s^{3} + 3s^{4} + s^{5}$$
(14)



Figure 3: Kharitonov rectangles of interval polynomial (13) for $\omega \in \langle 0; 3 \rangle$



Figure 4: Kharitonov rectangles of interval polynomial (13) – detailed view

Furthermore, suggested simple graphical procedure for checking robust stability can be improved by finding of some finite precomputable frequency (so-called cutoff frequency) at which the frequency sweep can be terminated, i.e. the graphical test concluded (Barmish 1994).

THE OVERBOUNDING METHOD

However, it remains true that the interval uncertainty structure is considerably idealized and restrictive state because uncertain parameters typically enter into more than the only one coefficient (e.g., even an interval system in closed control loop leads, except for some specific cases, to the closed-loop characteristic polynomial with affine linear structure of uncertainty). In spite of that, the tools for robust stability analysis of interval systems can be utilized also for these more general events as an alternative to "their own" more general results. That is, complicated uncertainty structure can be "overbounded" by the interval one and this new family is sequentially tested. Unfortunately, this method brings into the analysis certain degree of conservatism due to ignoring of mutual dependencies among coefficients in the original family. As a result, robust stability is investigated only with sufficient (i.e. stronger) and not necessary and sufficient condition.

The preceding consideration is demonstrated on example from (Barmish 1994). The family of polynomials (with multilinear uncertainty structure) is described by:

$$p(s,q) = s^{4} + (5 + 0.2q_{1}q_{2} + 0.1q_{1} - 0.1q_{2})s^{3} + (6 + 3q_{1}q_{2} - 4q_{2})s^{2} + (6 + 6q_{1} - 8q_{2})s + (15) + (0.5 - 3q_{1}q_{2})$$

and uncertainty bound $|q_i| \le 0.25$ for i = 1, 2. The objective is to determine whether p(s,q) is robustly stable. New bounds can be computed as:

$$\begin{array}{l}
 q_{0}^{-} = \min_{q \in Q} a_{0}(q) = \min_{-0.25 \le q_{1} \le 0.25} \left(0.5 - 3q_{1}q_{2} \right) = 0.3125 \\
 \overline{q}_{0}^{+} = \max_{q \in Q} a_{0}(q) = \max_{-0.25 \le q_{1} \le 0.25} \left(0.5 - 3q_{1}q_{2} \right) = 0.6875 \\
 \overline{q}_{1}^{-} = \min_{q \in Q} a_{1}(q) = \min_{-0.25 \le q_{1} \le 0.25} \left(6 + 6q_{1} - 8q_{2} \right) = 2.5 \\
 \overline{q}_{1}^{+} = \max_{q \in Q} a_{1}(q) = \max_{-0.25 \le q_{1} \le 0.25} \left(6 + 6q_{1} - 8q_{2} \right) = 9.5
\end{array}$$
(16)

Analogical computations yield to the coefficients $\overline{q_2} = 4.8125$, $\overline{q_2} = 7.1875$, $\overline{q_3} = 4.9475$, $\overline{q_3} = 5.0375$. The overbounding interval family of polynomials is given by:

$$\overline{p}(s, \overline{q}) = s^4 + [4.9475, 5.0375]s^3 + + [4.8125, 7.1275]s^2 + [2.5, 9.5]s + (17) + [0.3125, 0.6875]$$

By applying the Kharitonov theorem or graphical test, it is straightforward to verify that the family (17) is robustly stable. Therefore, it can be concluded that the original family (15) must also be robustly stable. Thus, the overbounding method has been successful in this case.

However, one has to be careful here. As it was adumbrated hereinbefore, if the new overbounding family was not robustly stable, it could not to be decided about the authentic family, i.e. although the Kharitonov rectangles would cover the origin of the complex plane, the value sets of the original family would not necessarily have to include it. This is illustrated in next example (Šebek 2009), where the polynomial family (with affine linear uncertainty structure) is given by:

$$p(s,q) = s^{4} + (2q_{2}+1)s^{3} + (2q_{1}-q_{2}+4)s^{2} + (q_{2}+1)s + (q_{1}-2q_{2}+2)$$
(18)

with uncertainty bounds $q_1 \in \langle -0.5, 2 \rangle$, $q_2 \in \langle -0.3, 0.3 \rangle$. The overbounding interval polynomial is then:

$$\overline{p}(s,\overline{q}) = s^4 + [0.4, 1.6]s^3 + [2.7, 8.3]s^2 + + [0.7, 1.3]s + [0.9, 4.6]$$
(19)

As can be easily verified by the Kharitonov theorem, the overbounding family (19) is not robustly stable so it can not be said anything about robust stability of (18) and it has to be tested with the assistance of a more advanced method, i.e. the overbounding method is unsuccessful here. Apropos, the family (18) is robustly stable in fact.

CONCLUSION

The principal aim of the contribution has been to present the advantages and restrictions which arise during use of interval uncertainty. In addition to this, it has clarified the origin of uncertainties and it has shown their possible integration into mathematical model of controlled system. The paper has described the main tools of robust stability analysis, such as Kharitonov theorem, the value set concept and the zero exclusion condition, using the necessary theoretical background and consequently some illustrative examples. The final part is dedicated to usefullness of the methods also for, in practice very common, structures which are more complicated than only interval ones.

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LOCAL MODEL NETWORKS FOR MODELLING AND PREDICTIVE CONTROL OF NONLINEAR SYSTEMS

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KEYWORDS

Predictive control, Local Model Networks, Heatexchanger, Optimization.

ABSTRACT

The paper deals with the problem of modelling and control using the Local Model Network (LMN). The idea is based on development of multiple local models for the whole operating range of the controlled process. The local models are then smoothly connected using the validity or weighting functions to provide a nonlinear global model of the plant. For saving the computational load, linear model is obtained by interpolating the parameters of local models at each sample instant and then used in Model Predictive Control (MPC) framework to calculate the future behaviour of the process. The supervisory program, based on a nonlinear global model, computes desired values of manipulated variables leading to minimum utility consumption. The approach is verified in a control of model of a heat exchanger.

INTRODUCTION

Many of the processes in the chemical industry exhibit nonlinear behaviour. Their nonlinearities arise from the dynamics in chemical reactions, thermodynamic relationships, etc. Such processes are difficult to model and control. For such problems, there is a strong intuitive appeal in building systems which operate over a wide range of operating conditions by decomposing them into a number of simpler linear modelling or control problems. Multiple-model approaches for the modelling and control of nonlinear systems were proposed in the last decade (Murray-Smith and Johansen, 1997). Here local models are identified over the operating range of the process and form a global nonlinear model process by incorporating the validity function for each of these models (Johansen and Foss 1995).

The basic principles of this modelling approach have been more or less independently developed in different disciplines like neural networks, fuzzy logic, statistics and artificial intelligence with different names such as local model networks (Johansen and Foss 1993), Takagi–Sugeno fuzzy model (Takagi and Sugeno 1985) or neuro-fuzzy model (Narendra and Parthasarathy 1990; Zhang and Morris 2002). Similarities and differences between the LMN, radial basis function network (RBFN), fuzzy and Gaussian process model can be found in (Gregorcic and Lightbody 2008).

Model Based Predictive Control (MBPC) or only Predictive Control is one of the control methods which have developed considerably over a few past years. The main advantage of this methodology is that it enables a simple treatment of input and output constraints (Maciejowski 2002), and copes in a natural way with multivariable systems.

There are two ways to design controllers for local model structures, the linearization based and the local model-based approach. For linearization-based approach the local model network is linearized at the current operating point and linear controller is designed. The linearization of the LM network is very simple due to the structure of the model. In the second realisation a local controller is designed for each local model and the control output is then calculated as an interpolation of the local controller according to the current operating point. Both realisations have been widely used in the literature for control of nonlinear systems (Johansen et al., 2000;Mollov et all. 1999).

In this paper the operating regions are distributed in the operating space using the steady-state characteristic of the process. The data for identification of the local models were created by application perturbations around the chosen operating points. The local models were identified using the least-squared method. The parameters of the validity functions were then optimized by minimizing the output error. Thus a nonlinear global model of the process was obtained. Predictive control strategy that uses parameters obtained from linearization of the global model was then applied to provide set point tracking of the output of the plant.

The paper is organized as follows: Section II presents an overview of the local model network approach. The basics of Model Predictive Control are outlined in Section III. In Section IV, the heat-exchanger process is described. Section V describes the modelling of a heatexchanger using the LMN approach. In Sections VI a VII results of predictive control with and without the utility costs taken into consideration are presented.

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LOCAL MODEL NETWORKS

The basics of Local Model Networks approach are to decompose the operating space into zones where linear models are adequate approximations of dynamic behaviour within that regime, with a trade-off between the number of regimes and the accuracy of the global model. The architecture of LMN benefits from being able to incorporate the a priori knowledge about the system and conventional system identification methodology. The LMN structure also gives transparent and simple representation of the nonlinear system.

In the LMN representation, each model is a local approximation of the modelling surface over a subspace of the operating space, which can be seen as an operating regime (Figure 1).



Figure 1: The nonlinear input/output approximation (c) is obtained by combining three linear models (a) with validity functions (b)

If linear local models are assumed, the structure of the *i*-th submodel can be defined as follows:

$$\hat{y}_{i}(k) = -a_{i1}y(k-1) - a_{i2}y(k-2) - \dots - a_{in}y(k-n) + b_{i1}u(k-1) + b_{i2}u(k-2) + \dots + b_{n}^{i}u(k-m) (1) + d_{i} + \eta(k)$$

where *n* and *m* are the numbers of delayed input and output samples, is the d_i offset term, and $\eta(k)$ is assumed to be white noise. Eq. 1 can be rewritten to regression form:

$$\hat{y}_i(k) = \boldsymbol{\psi}(k-1)^T \boldsymbol{\Theta}_i + \eta(k)$$
(2)

where the repressor vector $\psi(k-1)$ is given as

and the vector of parameters as:

 $\psi(k-$

$$\boldsymbol{\mathcal{P}}_{i} = \begin{bmatrix} a_{i1}, \dots, a_{in}, b_{i1}, \dots, b_{im}, d_{i} \end{bmatrix}$$
(4)

The LMN structure can then be represented as follows:

$$\hat{y}(k+1) = \sum_{i=1}^{M} \varphi_i(\boldsymbol{\phi}(k)) \boldsymbol{\psi}(k)^T \boldsymbol{\Theta}_i$$
(5)

The validity functions $\varphi_i(k)$ are functions of some scheduling vector $\phi(k)$. The scheduling vector, which defines the operating point of the system, can include any system state or variable. Although any function

with locally limited activation might be applied as a validity function, a common choice is Gaussian or a B-Spline function. The Gauss function for *i*-th model is given by

$$\tilde{\varphi}_{i}(\boldsymbol{\phi}(k)) = \exp\left(-\frac{1}{2}\left(\boldsymbol{\phi}-\boldsymbol{c}_{i}\right)^{T}\boldsymbol{\sigma}_{i}^{-2}\left(\boldsymbol{\phi}-\boldsymbol{c}_{i}\right)\right) \qquad (6)$$

The validity functions are generally normalized:

$$\varphi_i(\boldsymbol{\phi}(k)) = \frac{\tilde{\varphi}_i(\boldsymbol{\phi}(k))}{\sum_{i=1}^{M} \tilde{\varphi}_i(\boldsymbol{\phi}(k))}$$
(7)

Normalization of the validity functions is often motivated by the desire to achieve a partition of unity. By partition of unity it is meant that at any point in the input space sum of all normalized validity functions equals unity, i.e.

$$\sum_{i=1}^{M} \varphi_i(\boldsymbol{\phi}) = 1 \tag{8}$$

However, normalization also leads to a number of other important side-effects that have consequences for the resulting network (Shorten and Murray-Smith 1997).

Assuming that both the validity functions of the LMN and the parameters of the local model there are known there are two ways of interpolating between the local models:

• A weighted sum of the outputs of local models is used to produce an output of the LMN (Figure 2)

• Assuming all the local models have the same structure parameters of the local models are blended to form an LMN

The blending of parameters provides better transparency, however, cannot be used in applications where the structure of the local models changes across the operating space.



Figure 2: Local model network structure

MODEL PREDICTIVE CONTROL

In general, industrial processes are nonlinear, but most MPC applications are based on the use of linear models. The first reason is that identification of a linear model is relatively simple and the linear models are sufficient when the plant is operating in the neighbourhood of the operating point. Secondly, the use of linear models with quadratic objective function gives rise to a convex problem which can be solved by Quadratic Programming.

If all of the local models share the same structure across the operating space, the parameters of the local models can be blended:

$$\hat{y}(k+1) = \boldsymbol{\psi}(k)^T \sum_{i=1}^M \varphi_i(\boldsymbol{\phi}(k))\boldsymbol{\Theta}_i + \eta(k)$$
(9)

The structure of the overall model in this case, remains the same as the structure of the individual local models. A predictor in a vector form is then given by

$$\hat{\boldsymbol{y}} = \boldsymbol{G} \Delta \boldsymbol{u} + \boldsymbol{Y} \tag{10}$$

where \hat{y} is a vector of system predictions along the prediction horizon N, Δu is a vector of control increments, Y is the free response vector. G is a dynamics matrix.

The computation of a control law of MPC is based on minimization of the following criterion

$$J = \sum_{j=1}^{N} \left\| \hat{y}(k+j|k) - w(k+j) \right\|_{Q}^{2} + \sum_{j=1}^{N} \left\| \Delta u(k+j-1) \right\|_{R}^{2}$$
(11)

where $\hat{y}(k+j|k)$ is a *j* steps ahead prediction of the system, w(k+j) is a future reference trajectory and Q, R are the positive definite weighting matrices.

The reference trajectory vector

$$\boldsymbol{w} = [w(k+1), \dots, w(k+N)]^T$$
(12)
is obtained from the first-order lag system:

$$w(k) = \alpha w(k-1) + (1-\alpha)\omega$$
(13)

where α is an adjustable parameter of the reference trajectory and ω is the output set point.

The criterion 11 can be rewritten to more general matrix form:

$$J(k,N) = \left(\boldsymbol{w} - \hat{\boldsymbol{y}}\right)^T \boldsymbol{Q} \left(\boldsymbol{w} - \hat{\boldsymbol{y}}\right) + \Delta \boldsymbol{u}^T \boldsymbol{R} \Delta \boldsymbol{u} \qquad (14)$$

Using the expression (10) it can be simplified

$$J(k,N) = \Delta u^{2} H \Delta u + 2g^{2} \Delta u + f \qquad (15)$$

where the gradient g and the Hess matrix H are defined by following expressions

$$H = G^{T} QG + R$$

$$g = (Y - w)^{T} QG$$
(16)

$$f = (w - Y)^{T} Q(w - Y)$$

Since the vector f is a constant vector it does not have an effect on the quadratic programming results. The constraints for the control signal and control signal increments are given:

$$A\Delta u \le b \tag{17}$$

$$\boldsymbol{A} = \begin{bmatrix} I_{u} \\ -I_{u} \\ I_{\Delta u} \\ -I_{\Delta u} \end{bmatrix} \quad \boldsymbol{b} = \begin{bmatrix} u^{\max} - Iu(k-1) \\ -u^{\min} + Iu(k-1) \\ \Delta u^{\max} \\ -\Delta u^{\min} \end{bmatrix}$$
(18)

Parameters u^{max} and u^{min} are constraints for the control signals and Δu^{max} and Δu^{min} are constraints for the control signal increments. Matrices I_u and $I_{\Delta u}$ are defined as:

$$I_{\Delta u} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \vdots \\ \vdots & 0 & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{bmatrix},$$
(19)
$$I_{u} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 1 & 1 & 0 & \vdots \\ \vdots & 1 & \ddots & 0 \\ 1 & \cdots & 1 & 1 \end{bmatrix}.$$

DESCRIPTION OF THE PROCESS

Heat exchangers are widely used in space heating, petrochemical plants or power plants. It is represented by a vessel (see Figure 3) filled with water. It is possible to increase the water temperature with electric heating A. Heating power E is controlled continuously. Cooling helix B is used to decrease water temperature T_C .



Figure 3 Scheme of a heat-exchanger

The system can be described under a simplified assumption (ideal mixing, characteristic temperatures, etc.) by 3 differential equations (Dusek and Honc 2009).

$$m_{A}c_{A}\frac{dT_{A}}{dt} = \alpha_{A}S_{A}\left(T_{c}-T_{A}\right) + E$$

$$m_{B}c_{B}\frac{dT_{B}}{dt} = \alpha_{B}S_{B}\left(T_{c}-T_{B}\right) + c_{B}Q(T_{B0}-T_{B})$$

$$m_{C}c_{C}\frac{dT_{C}}{dt} = \alpha_{A}S_{A}\left(T_{A}-T_{C}\right) + \alpha_{B}S_{B}\left(T_{B}-T_{C}\right)$$

$$+ \alpha_{C}S_{C}\left(T_{O}-T_{C}\right) + qc_{C}\left(T_{C0}-T_{C}\right)$$

$$(20)$$

 T_x are characteristic temperatures

 T_{B0} is input temperature of cooling helix

 T_0 is ambient temperature

 T_{C0} is input temperature

where

 m_x are masses

- c_x are specific heat capacities
- $S_{\rm x}$ are heat transfer areas
- $\alpha_{\rm x}$ are heat transfer coefficients.

The input variables are constrained – cooling water flow is within the range $0 \le Q \le Q_{\text{max}}$, and heating power $0 \le E \le E_{\text{max}}$.

The parameters of the system that are used in the simulations are given in Table 1

Table 1 Parameters of the system

Par.	Value	Par.	Value
m_A	0.5 kg	S_A	$0.0095 m^2$
m_{B}	0.1 kg	$S_{\scriptscriptstyle B}$	$0.065 m^2$
m_{C}	4.0 kg	S_{C}	$0.24 m^2$
C_A	$452 J k g^{-1} K^{-1}$	$\alpha_{_{A}}$	$750 Jm^{-2}s^{-1}K^{-1}$
C_B	4180 $Jkg^{-1}K^{-1}$	$\alpha_{\scriptscriptstyle B}$	$500 Jm^{-2}s^{-1}K^{-1}$
c_{c}	4180 $Jkg^{-1}K^{-1}$	α_{c}	$5 Jm^{-2}s^{-1}K^{-1}$
T_{C0}	25 °C	q	$0.0016 \ kgs^{-1}$
T_{B0}	$15 {}^{0}C$	T_0	25 °C
E_{\min}	$0 kgm^2 s^{-3}$	\mathcal{Q}_{\min}	$0 \ kgs^{-1}$
$E_{\rm max}$	$500 kgm^2 s^{-3}$	$Q_{\rm max}$	$0.0083 \ kgs^{-1}$

MODELLING OF HEAT EXCHANGER

The local modelling approach was used to model the dynamic and steady-state properties of the system. The process exhibits nonlinear behaviour as can be seen from steady-state characteristics depicted in Figure 4.



Figure 4. Steady-state characteristics of the heat exchanger

Five separate sets of data were collected at different operating points. The operating points were chosen at the corners of the operating region and in the centre of it. Each data set is restricted to be close to the locus of equilibrium points. To get representative data for each subspace, an additional low-amplitude excitation signal has to be injected into the system. In this way the system is excited locally at the particular operating point and the collected data will reflect the dynamic which is a valid representation of the system only on the subspace close to operating point. Away from those points the accuracy of the network can decrease rapidly due to unmodelled off-equilibrium dynamics.

At each chosen point an affine ARX model

 M_i : $y_i(k+1) = b_1u_1(k) + b_2u_2(k) + ay(k) + c$ (21) was identified. The scheduling vector $\phi(k)$ contains the values of input $u_1(k-1)$ and y(k-1). The widths of the Gaussian validity functions σ_i^{-2} were optimized by minimization of a mean-squared modelling error over the training data using the criterion:

$$J = \frac{1}{N} \sum_{k=1}^{N} \left(y(k) - \hat{y}(k) \right)^2$$
(22)

It is important to highlight here that in many industrial applications it could be difficult or even unsafe to drive the system rapidly across the operating space and hence global data is often not available. The modelling performance of the LMN is shown in Figure 5 where step changes of both inputs are applied to the system being modelled and LMN.



Figure 5. Comparison of the measured output of system (green) and output of the LMN (red)



Figure 6. Steady-state characteristics of the LMN

Since the LMN will be used for finding the optimal inputs the steady-state properties of the LMN are of high importance. The steady-state characteristic of the LMN is depicted in Figure 6.

PREDICTIVE CONTROL OF THE HEAT **EXCHANGER MODEL**

The control task is to control the temperature inside the vessel $y(k) = T_c(k)$ by manipulating the flow-rate of the cooling water $u_1(k) = Q(k)$ and heating power $u_2(k) = E(k)$. The length of prediction horizon, was set to N = 20 with sampling period of 1 minute. The weighting matrices Q, S were chosen as

$$Q = 3I$$

$$S = \begin{bmatrix} S_{1} & 0 & \cdots & 0 \\ 0 & S_{1} & 0 \\ \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & S_{1} \end{bmatrix}$$

$$S_{1} = \begin{bmatrix} 1000 & 0 \\ 0 & 0.1 \end{bmatrix}$$

$$S_{1} = \begin{bmatrix} 1000 & 0 \\ 0 & 0.1 \end{bmatrix}$$

$$Q = 3I$$

$$S_{1} = \begin{bmatrix} 1000 & 0 \\ 0 & 0.1 \end{bmatrix}$$

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$$S_{1} = \begin{bmatrix} 1000 & 0 \\ 0 & 0.1 \end{bmatrix}$$

$$S_{1} = \begin{bmatrix} 1000 & 0 \\ 0 & 0.1 \end{bmatrix}$$

200 Figure 7 Control of a heat exchanger

100

Figure 7 shows the dynamic responses of the system when the sequence of changes is introduced into the

400

Time [min]

500

600

700

800

300

system. The heating and cooling act against each other. As can be seen at the time from 100 to 300 minutes both inputs are active. The output temperature can be reach with an infinite number of combinations of inputs. However, only one combination of inputs has minimal utility costs.

PREDICTIVE CONTROL WITH MINIMAL COST

In the MPC strategy an extra term in the cost function of problem (14) is added to account for the utility cost. Thus, the control scheme uses two level structure that consists of supervisory level that determines the optimal steady-state inputs and MPC level that guides the process to this point. The optimization problem of the supervisory level is the minimization of the total utility consumption:

$$J(u_{1}, u_{2}) = c_{1}u_{1} + c_{2}u_{2}$$

subject to : (24)
 $L(u_{1}, u_{2}) = w(k + N)$

where c_1, c_2 are the cold and hot utility costs per unit and $L(u_1, u_2)$ represents the steady-state response of the system given the inputs u_1, u_2 .

The desired optimal values that are obtained at supervisory level are included in the cost function of the control problem as a new term that penalizes the distance that the system is from the desired condition. In (Dusek and Honc 2009) the difference between the optimal state and state at the end of horizon is used. Here the difference between the last control signal and optimal control signal is weighted in the criterion. The MPC optimization problem is reformulated as follows:

$$J(k,N) = (\mathbf{w} - \hat{\mathbf{y}})^{T} \mathbf{Q}(\mathbf{w} - \hat{\mathbf{y}}) + \Delta \mathbf{u}^{T} \mathbf{R} \Delta \mathbf{u} + (\mathbf{K} \Delta \mathbf{u} - \mathbf{l})^{T} \mathbf{S} (\mathbf{K} \Delta \mathbf{u} - \mathbf{l})$$
(25)

where matrix **K** and vector **l** are defined as:

$$\boldsymbol{K} = \begin{bmatrix} 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 1 & 0 & 1 & 0 & \dots & 1 & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 1 & 0 & 1 & \dots & 0 & 1 \end{bmatrix} \boldsymbol{I} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ u_{1optim} - u_1(k-1) \\ u_{2optim} - u_2(k-1) \\ u_{2optim} - u_2(k-1) \end{bmatrix}$$
(26)

Only the future final value is used in the criterion to separate the effect of the optimising action of the supervisory level from the more immediate MPC closed-loop corrections. Analysis of this technique concerning the model plant mismatch can be found in (Gonzales et al. 2006). The main control objective is to follow the set-point and respect manipulated variable constrains and at the same time to minimize energy costs for heating and cooling. The same horizons and weighting matrices as in the previous control have been used in the criterion. Additional weighting matrix S was chosen as

$$S = \begin{bmatrix} S_{1} & 0 & \cdots & 0 \\ 0 & S_{1} & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & S_{1} \end{bmatrix}$$
(27)
$$R_{1} = \begin{bmatrix} 1000 & 0 \\ 0 & 0.1 \end{bmatrix}$$

The prices utilities at the supervisory level control were set to $c_1 = 0.01$ and $c_2 = 1$ to reflect that prices for heating are much higher than prices for cooling. At each step change of reference value the optimal values of inputs with minimal utility costs are computed.



Figure 8 Control of a heat exchanger with minimal costs

As can be seen, now the cooling is used only for decreasing the temperature or if the setpoint temperature that is less then ambient temperature. The optimal input conditions are calculated based on an approximated non-linear model. The closer the non-linear model utilized in the steady-state optimization is from the process, the more consistent will be the targets and set points sent to the control system.

Despite of steady-state model mismatch, by penalizing only the last control action in the control horizon, the MPC remains free to use the remaining control actions to satisfy dynamic requirements and set point targets. The final response to the system with supervisory control for minimal utility costs is depicted in Figure 8.

CONCLUSION

In this paper, a MPC scheme based on local model network has been applied to model of a heat exchanger. The operation of the process is decomposed into a set of operating regimes, and simple local models are developed for each regime. These are combined into a global model structure using the validity functions. The supervisory level looks for steady-state input values in agreement with minimum utility consumption, while the MPC accounts for transient performance and offset free controlled outputs.

ACKNOWLEDGMENT

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NEURAL NETWORK PREDICTIVE CONTROL OF A CHEMICAL REACTOR

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KEYWORDS

Model predictive control, neural network, continuous stirred tank reactor.

ABSTRACT

Model Predictive Control (MPC) refers to a class of algorithms that compute a sequence of manipulated variable adjustments in order to optimize the future behaviour of a plant. MPC technology can now be found in a wide variety of application areas. The neural network predictive controller that is discussed in this paper uses a neural network model of a nonlinear plant to predict future plant performance. The controller calculates the control input that will optimize plant performance over a specified future time horizon. In the paper, simulation of the neural network based predictive control for the continuous stirred tank reactor is presented. The simulation results are compared with fuzzy and PID control.

INTRODUCTION

Conventional process control systems utilize linear dynamic models. For highly nonlinear systems, control techniques directly based on nonlinear models can be expected to provide significantly improved performance.

Model Predictive Control (MPC) concept has been extensively studied and widely accepted in industrial applications. The main reasons for such popularity of the predictive control strategies are the intuitiveness and the explicit constraint handling.

The predictive controllers are used in many areas, where high-quality control is required (Qin and Badgwell, 1996; Qin and Badgwell, 2000; Rawlings, 2000). Model-based predictive control refers to a class of control algorithms, which are based on a process model. MBPC can be applied to such systems as e.g. multivariable, non-minimum-phase, open-loop unstable, non-linear, or systems with long time delays. Constrained model predictive control becomes the standard algorithm for advanced control in process industries.

Several versions of MPC techniques are Model Algorithmic Control (MAC) (Richalet et al., 1978),

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) Dynamic Matrix Control (DMC) (Cutler and Ramaker, 1980), and Internal Model Control (IMC) (Garcia and Morari, 1982). Although the above techniques differ from each other in some details, they are fundamentally the same, because all of them are based on linear process modelling. If the nonlinear model is available, the computational requirements are expected to be very high (Garcia et al., 1989), especially for nonlinear MIMO processes. It is estimated that, in a typical commissioning project, modelling efforts can take up to 90% of the cost and time in implementing a model predictive controller (Morari and Lee, 1999).

The Neural Network Model Predictive Control (NNMPC) is another typical and straightforward application of neural networks to nonlinear control. When a neural network is combined with MPC approach, it is used as a forward process model for the prediction of process output (Hunt et al., 1992; Nørgaard et al., 2000).

Control of chemical reactors is one of the most studied areas of process control. In this paper, a neural network based predictive control strategy is applied to a continuous-time stirred reactor with two parallel firstorder irreversible exothermic reactions. Simulation results show that neural network based predictive control gives promising results.

MODEL-BASED PREDICTIVE CONTROL (MBPC)

MBPC is a name for several different control techniques. They all are associated with the same idea. The prediction is based on the model of the process.



Figure 1: Classical model-based predictive control scheme.

The target of the model-based predictive control is to predict the future behaviour of the process over a certain horizon using the dynamic model and obtaining the control actions to minimize a certain criterion, generally

$$J(k,u(k)) = \sum_{j=N_{i}}^{2} (y(k+j) - y_{r}(k+j))^{2} + \lambda \sum_{j=1}^{N_{u}} (u(k+j-1))^{2}$$
(1)

Signals y(k+j), yr(k+j), u(k+j) are *j*-step ahead predictions of the process output, the reference trajectory and the control signal, respectively. The values N_I and N_2 are minimal and maximal prediction horizons and N_u is the prediction horizon of control signal. The value of N_2 should cover the important part of the step response curve. The use of the control horizon N_u reduces the computational load of the method. The parameter λ represents the weight of the control signal. At each sampling period only the first control signal of the calculated sequence is applied to the controlled process. At the next sampling time the procedure is repeated. This is known as the receding horizon concept.

The controller consists of the plant model and the optimization block.

Eq. (1) is used in combination with input and output constraints:

$$u_{min} \leq u \leq u_{max}$$

$$\Delta u_{min} \leq \Delta u \leq \Delta u_{max}$$

$$y_{min} \leq y \leq y_{max}$$

$$\Delta y_{min} \leq \Delta y \leq \Delta y_{max}$$
(2)

The ability to handle constraints is one of the key properties of MBPC and also caused its spread, use, and popularity in industry.

MBPC algorithms are reported to be very versatile and robust in process control applications.

NEURAL NETWORK PREDICTIVE CONTROL

Neural networks have been applied very successfully in the identification and control of dynamic systems. The universal approximation capabilities of the multilayer perceptron make it a popular choice for modelling of nonlinear systems and for implementing of nonlinear controllers.



Figure 2: Neural network as a function approximator.

The unknown function may correspond to a system we are trying to control, in which case the neural network will be the identified plant model.

Two-layer networks, with sigmoid transfer functions in the hidden layer and linear transfer functions in the output layer, are universal approximators (Figure 2).

The prediction error between the plant output and the neural network output is used as the neural network training signal. The neural network plant model uses previous inputs and previous plant outputs to predict future values of the plant output. The structure of the neural network plant model is given in the following figure, where u(k) is the system input, $y_p(k)$ is the plant output, the blocks labelled TDL are tapped delay lines that store previous values of the input signal, $IW^{i,j}$ is the weight matrix from input number *j* to layer number *i*. $LW^{i,j}$ is the weight matrix from layer number *j* to layer number *i*.



Figure 3: Structure of the neural network plant model.

This network can be trained off-line in batch mode, using data collected from the operation of the plant.

The procedure for selecting the network parameters is called training the network. The Levenberg-Marquardt (LM) algorithm is very efficient for training. The LM algorithm is an iterative technique that locates the minimum of a function that is expressed as the sum of squares of nonlinear functions. It has become a standard technique for nonlinear least-squares problems and can be thought of as a combination of steepest descent and the Gauss-Newton method (Levenberg, 1944; Madsen *et al.*, 2004; Marquardt, 1963; Mittelmann, 2004, Kelley, 1999).

When the current solution is far from the correct one, the algorithm behaves like a steepest descent method: slow, but guaranteed to converge. When the current solution is close to the correct solution, it becomes a Gauss-Newton method.

Let f be an assumed functional relation which maps $p \in \mathbb{R}^m$ a parameter vector to an estimated measurement vector $\hat{x} = f(p), \hat{x} \in \mathbb{R}^n$. An initial parameter estimate p0 and a measured vector x are provided and it is desired to find the vector p^+ that best satisfies the functional relation f, i. e. minimizes the squared distance $e^T e$ with $e = x - \hat{x}$. The basis of the LM algorithm is a linear approximation to f in the neighbourhood of **p**. For a small $\|\delta_p\|$, a Taylor series expansion leads to the approximation $f(p+\delta_p) \approx f(p) + J\delta_p$, where **J** is the Jacobian matrix $\frac{\partial f(p)}{\partial p}$. Like all non-linear optimization methods, LM is iterative: initiated at the starting point p_0 , the method produces a series of vectors p1, p2, ..., that converge towards a local minimizer p^+ for f. Hence, at each step, it is required to find the δ_p that minimizes the quantity $||e-J\delta_p||$. The sought δ_p is thus the solution of a linear least-square problem: the minimum is attained when $J\delta_p - e$ is orthogonal to the column space of **J**. This leads to $J^T (J\delta_p - e) = 0$, which yields δ_p as the solution of the normal equations:

$$J^T J \delta_p = J^T e.$$
 (3)

The matrix $J^T J$ in the left hand side of Eq. (3) is the approximate Hessian, i.e. an approximation to the matrix of second order derivatives. The LM method actually solves a slight variation of Eq. (3), known as the augmented normal equations $N\delta_p = J^T e$, where the offdiagonal elements of N are identical to the corresponding elements of $J^T J$ and the diagonal elements are given by $N_{ii} = \mu + [J^T J]_{ii}$ for some $\mu > 0$. The strategy of altering the diagonal elements of $J^T J$ is damping and μ is referred to the damping term. If the updated parameter vector $P^{+\delta}_{p}$ with δ_{p} computed from Eq. (3) leads to a reduction of the error e, the update is accepted and the process repeats with a decreased damping term. Otherwise, the damping term is increased, the augmented normal equations are solved again and the process iterates until a value δ_p of that decreases error is found.

In LM, the damping term is adjusted at each iteration to assure a reduction in the error e. The LM algorithm terminates when at least one of the following conditions is met:

• The magnitude of the gradient of $e^{T}e$, i.e. $J^{T}e$ in the right hand side of Eq. (3), drops below a threshold $\varepsilon \varepsilon_1$.

- The relative change in the magnitude of δ_p drops below a threshold $\epsilon 2$.
- The error $e^{T}e$ drops below a threshold $\varepsilon 3$.

• A maximum number of iterations k_{max} is completed.

If a covariance matrix Σ for the measured vector x is available, the minimum is found by solving a weighted least squares problem defined by the weighted normal equations

$$J^T \sum J\delta_p = J^T \sum e \tag{4}$$

FUZZY CONTROL

Classic control theory is usually based on mathematical models which describe the behaviour of the process under consideration. The main aim of fuzzy control is to simulate a human expert (operator), who is able to control the process by translating the linguistic control rules into a fuzzy set theory.

In 1965 Lotfi A. Zadeh introduced fuzzy sets, where a more flexible sense of membership is possible. The past few years have witnessed a rapid growth in the use of fuzzy logic controllers for the control of processes that are complex and badly defined. Most fuzzy controllers developed till now have been of the rule-based type (Driankov et al., 1993), where the rules in the controller attempt to model the operator's response to particular process situations. An alternative approach uses fuzzy or inverse fuzzy model in process control (Babuška *et al.*, 1995; Jang 1995) because it is often much easier to obtain information on how a process responds to particular inputs than to record how, and why, an operator responds to particular situations.

A review of the work on fuzzy control has been presented by Lee (Lee 1990).

Design of a simple fuzzy controller can be based on a three step design procedure, that builds on PID control: start with a PID controller, insert an equivalent, linear fuzzy controller and make it gradually nonlinear. A fuzzy controller can include empirical rules, and that is especially useful in operator controlled plants. Take e.g. a typical fuzzy controller:

- if error is negative and change in error is negative then output is negative big,
- if error is negative and change in error is zero then output is negative medium.

The collection of rules is called a rule base. The computer is able to execute the rules and compute a control signal depending on the measured inputs error and change in error. The inputs are most often hard or crisp measurements from some measuring equipment.

A dynamic controller would have additional inputs, for example derivatives, integrals, or previous values of measurements backwards in time.

The block fuzzification converts each piece of input data to degrees of membership by a lookup in one or several membership functions.

The rules may use several variables both in the condition and the conclusion of the rules. Basically a

linguistic controller contains rules in the if-then format, but they can be presented in different formats.

The resulting fuzzy set must be converted to a number that can be sent to the process as a control signal. This operation is called defuzzification. There are several defuzzification methods. Output scaling is also relevant. In case the output is defined on a standard universe this must be scaled to engineering units.



Figure 4: Fuzzy controller

Takagi-Sugeno type controller

The output sets can often be linear combinations of the inputs, or even a function of the inputs. The developed Fuzzy Logic Toolbox for the software package Matlab implements one of the hybrid schemes known as the Adaptive Network based Fuzzy Inference System (Anfis). Anfis represents a Sugeno-type fuzzy system in a special five-layer feed forward network architecture and uses a hybrid learning algorithm to identify the membership function parameters of single-output, Sugeno type fuzzy inference systems. Suppose the rule base of a Sugeno - Takagi fuzzy system is as follows (Nauck *et al.*, 1977; Takagi *et al.*, 1985.):

if x_1 is A_i and x_2 is B_i then $y=p_i x_1 + q_i x_2 + r_i$, i=1,..N(5)

The if-parts (antecedents) of the rules describe fuzzy regions in the space of input variables error e, its derivative de and the then-parts (consequents) are functions of the inputs, usually linear with consequent parameters p_i , q_i , r_i , y is an output variable, A_i , B_i are fuzzy sets characterized by three linguistic variables (small, middle, large).

SIMULATIONS AND RESULTS

Chemical reactor

Consider a continuous stirred tank reactor (CSTR) (Vasičkaninová and Bakošová, 2005; Vasičkaninová and Bakošová, 2006) with two parallel first-order irreversible reactions according to the scheme $A \xrightarrow{k_1} B A \xrightarrow{k_2} C$. The measured and controlled

output is the temperature of the reaction mixture. The control input is the volumetric flow rate of the cooling medium.

The simplified non-linear dynamic mathematical model of the chemical reactor consists of five differential equations:

$$\frac{dc_A}{dt} = \frac{q}{V} c_{AV} - \frac{q}{V} c_A - k_1 c_A - k_2 c_A \tag{6}$$

$$\frac{dc_B}{dt} = \frac{q}{V} c_{Bv} - \frac{q}{V} c_B + k_I c_A \tag{7}$$

$$\frac{dc_C}{dt} = \frac{q}{V} c_{CV} - \frac{q}{V} c_C + k_2 c_A \tag{8}$$

$$\frac{dT}{dt} = \frac{q}{V}T_v - \frac{q}{V}T - \frac{Ak}{V\rho C_p} \left[T - T_c\right] + \frac{\hat{Q}_r}{V\rho C_p} \tag{9}$$

$$\frac{dT_c}{dt} = \frac{q_c}{V_c} T_{vc} - \frac{q_c}{V_c} T_c + \frac{Ak}{V_c \rho_c C_{pc}} \left[T - T_c \right] \quad (10)$$

The reaction rate coefficients are non-linear functions of the reaction temperature being defined by the Arrhenius relations

$$k_1 = k_{10}e^{-\frac{E_1}{RT}} \quad k_2 = k_{20}e^{-\frac{E_2}{RT}} \tag{11}$$

The heat generated by chemical reactions is expressed as

$$\dot{\mathcal{Q}}_r = k_1 c_A V \left(-\varDelta_r H_1\right) + k_2 c_A V \left(-\varDelta_r H_2\right) \quad (12)$$

Here, *c* are concentrations, *T* are temperatures, *V* are volumes, ρ are densities, *Cp* are specific heat capacities, *q* are volumetric flow rates, $\Delta_r H$ are reaction enthalpies, *A* is the heat transfer area, *k* is the heat transfer coefficient. The subscript *c* denotes the coolant, *r* the reacting mixture and the superscript *s* denotes the steady-state values in the main operating point. Parameters and inputs of the reactor are enumerated in Table 1.

Table 1: Reactor parameters and inputs

q= 0.015 m ³ min -1	$\Delta_r H_1 = -8.6.10^4 \text{ kJ kmol} -1$
V=0.23 m ³	$\Delta_r H_2 = -1.82.10^4 \text{ kJ kmol}$
$V_c = 0.21 m^3$	-1
ρ =1020 kg m ⁻³	$c_{Av} = 4.22 \text{ kmol m}^{-3}$
$\rho_c=998 \text{ kg m}^{-3}$	$c_{Bv} = 0 \text{ kmol m} -3$
Cp=4.02 kJ kg ⁻¹ K ⁻¹	$c_{Cv} = 0 \text{ kmol m}^{-3}$
Cpc= 4.182 kJ kg ⁻¹	$T_v = 328 \text{ K}$
K-1	$T_{cv} = 298 \text{ K}$
A=1.51 m ²	$q^{s}c = 0.004 \text{ m}^{3} \text{ min}^{-1}$
k=42.8 kJm	$T^{S} = 363.61 K$
-2_{\min} -1K-1	$T^{s}c = 350.15 \text{ K}$
k10=1.55.10 ¹¹ min ⁻¹	$c^{s} A = 0.4915$ kmol m $^{-3}$
k20=4.55.10 ²⁵ min ⁻¹	

E ₁ /R=9850 K	$c^{s}B = 2.0042 \text{ kmol m}^{-3}$
E ₂ /R=22019 K	$c_{C}^{s} = 1.7243$ kmol m $^{-3}$

The reactions in the described reactor are exothermic ones and the heat generated by the chemical reactions is removed by the coolant in the jacket of the tank. The control objective is to keep the temperature of the reacting mixture close to a desired value.

Neural Network Model Predictive Control of the CSTR

The designed controller uses a neural network model to predict future CSTR responses to potential control signals. An optimization algorithm then computes the control signals that optimize future plant performance. The neural network plant model was trained using the Levenberg-Marquardt algorithm. The training data were obtained from the nonlinear model of the CSTR (6)-(10).

The used model predictive control method was based on the receding horizon technique. The neural network model predicted the plant response over a specified time horizon. The predictions were used by a numerical optimization program to determine the control signal that minimizes the following performance criterion over the specified horizon.

$$J(k,u(k)) = \sum_{j=N_{1}}^{N_{2}} (y_{m}(k+j) - y_{r}(k+j))^{2} + \lambda \sum_{j=1}^{N_{u}} (u'(k+j-1) - u'(k+j-2))$$
(13)

where N_1 , N_2 , and N_u define the horizons over which the tracking error and the control increments are evaluated. The *u'* variable is the tentative control signal, y_r is the reference response, and y_m is the network model response. The λ value determines the contribution that the sum of the squares of the control increments has on the performance index (Demuth and Beale, 2002). The controller block was implemented in Simulink. Constraints and parameters values: $0 \le u \le 0.02$, $354 \le y_p \le 365$, NI = 1, N2 = 7, Nu = 3, $\lambda = 0.5$.



Figure 5: Neural Network Predictive Control.

Model based predictive control was simulated and the comparison with a fuzzy controller and PID controller was also made.

Takagi-Sugeno controller for the CSTR

f

Sugeno-type fuzzy inference system was generated using subtractive clustering in the form:

if
$$e$$
 is A_i and de is B_i then $u = p_i e + q_i de + r_i$,

i=1, ... 3 (14) where *e* is the control error, *de* is the derivation of the control error, *u* is the calculated control input $q_c(t)$ and p_i , q_i , r_i are consequent parameters. The symmetric Gaussian function (*gaussmf* in MATLAB) was chosen as the membership function and it depends on two parameters σ and *c* as it is seen in (14)

$$(x;\sigma,c) = e^{\frac{-(x-c)^2}{2\sigma^2}}$$
(15)

The parameters σ and *c* for *gaussmf* are listed in the Table 2. For obtaining of these parameters, it was necessary to have the data sets of *e*, *de* and *u* at first. These data were obtained by simulation of PID control of the CSTR. The consequent parameters in the control input rule (14) are listed in Table 3 and the resulting plot of the output surface of a described fuzzy inference system is presented in Figure 6.

Table 2: Gaussian curve	e membership	functions
param	eters.	

e		de	
σ_i	ci	σ_i	ci
0,52	0,0018	0,53	0,0345
0,52	-0,0839	0,53	0,0003
0,52	-0,0665	0,53	0,0066

Table 3: Consequent parameters

pi	q_i	r _i
-0,256 -3,910	-0,092 -1,299	4,04 -156,12
-6,562	-2,517	151,33



Figure 6: Takagi-Sugeno controller - control signal *u* as function of control error *e* and its derivation *de*.

The feedback PID controllers were tuned by various methods (Ogunnaike and Ray, 1994) and the best simulation results were obtained with PID controller tuned using Chien-Hrones-Reswick method and its parameters are $K_C = -0.003$, $T_I = 16.8$, $T_D = 1.41$.

Figure 7 presents the simulation results of the predictive control of the CSTR. These results are compared with those obtained by fuzzy control and PID control of the CSTR.



Figure 7: Comparison of fuzzy and neural network predictive control of a CSTR with PID control.

The step changes of the reference *yr* were generated and the MBP, fuzzy and PID controllers were compared using the well-known *iae* criterion described as follows:

$$iae = \int_{0}^{1} (e) dt$$
 (16)

The iae values are given in Table 4.

Table 4: Comparison of the simulation results by integrated absolute error.

control method	iae
predictive control	174
fuzzy control	208
PID control	219

CONCLUSIONS

In this paper, an application of a neural network based predictive control strategy to a CSTR is presented. The simulation results confirmed that neural network based predictive control is one of the possibilities for successful control of CSTRs. The advantage of this approach is that it is not linear-model-based strategy and the control input constraints are directly included to the synthesis. Comparison of the MBPC simulation results with fuzzy control and classical PID control demonstrates the effectiveness and superiority of the proposed approach. Used fuzzy controller is simple, but it can lead to the nonzero steady-state control errors.

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SIMULATION OF ROBUST STABILIZATION OF A CHEMICAL REACTOR

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KEYWORDS

CSTR, multiple steady states, stabilization, static output feedback, PID controller.

ABSTRACT

The paper presents simulation experiments on the continuous stirred tank reactor for hydrolysis of propylene oxide to propylene glycol. The reactor is exothermic one. There are two parameters with only approximately known values in the reactor. These parameters are the reaction rate constant and the reaction enthalpy. The simplified mathematical model of the reactor consists of four nonlinear ordinary differential equations. The steady state analysis shows the reactor has multiple steady states and the open-loop analysis confirms that the reactor is open-loop unstable around one of these steady states. Then the possibility to stabilize the reactor using static output feedback PI and PID controllers is studied. Because of the presence of uncertainty in the continuous stirred tank reactor, the robust static output feedback is designed. Simulations are used for testing the stabilizability of the reactor around its open-loop unstable steady state.

INTRODUCTION

Continuous stirred tank reactors (CSTRs) are often used plants in chemical industry and especially exothermic CSTRs are very interesting systems from the control viewpoint because of their potential safety problems and the possibility of exotic behaviour such as multiple steady states, see e.g. (Molnár et al., 2002), (Pedersen and Jørgensen, 1999). Furthermore, operation of chemical reactors is corrupted by many different uncertainties. Some of them arise from varying or not exactly known parameters, as e.g. reaction rate constants, reaction enthalpies and heat transfer coefficients (Antonelli and Astolfi, 2003). The other control problems are due to the high sensitivity of the state and output variables to input changes and process nonlinearites (Alvarez-Ramirez and Femat, 1999). Operating points of reactors change in other cases. In addition, the dynamic characteristics may exhibit a varying sign of the gain in various operating points. All these problems can cause poor performance or even instability of closed-loop control systems.

Conventional control strategies, which are often used for reactor control design, can fail for such complicated systems and their effective control requires application some of advanced methods, as e. g. adaptive control (Vojtesek and Dostal, 2008), predictive control (Figueroa et al., 2007), robust control (Alvarez-Ramirez and Femat, 1999), (Gerhard et al., 2004), (Bakošová et al., 2005), (Tlacuahuac et al., 2005) and others.

Robust control has grown as one of the most important areas in modern control design since works by (Doyle and Stein, 1981), (Zames and Francis, 1983) and many others. One of the solved problems is also the problem of robust static output feedback control (RSOFC), which has been till now an important open question in control engineering, see e.g. (Syrmos et al., 1997), (Antonelli and Astolfi, 2003). Recently, it has been shown that an extremely wide array of robust controller design problems can be reduced to the linear matrix inequalities (LMIs) problem. Especially, the LMIs in semi-definite programming attract a big interest because of their ability to describe non-trivial control design problems integrating various specifications such as robustness, structural and performance constraints, as well as their suitability for efficient numerical processing through various available solvers, see e.g. (Boyd et al., 1994) and references therein.

From the system theory viewpoint, CSTRs belong to a class of nonlinear lumped parameter systems. Their mathematical models are described by sets of nonlinear ordinary differential equations (ODEs). The methods of modelling and simulation of such processes are described e. g. in (Ingham et al., 1994). The models are often used for a preliminary analysis of the steady-state, open-loop and closed-loop behaviour of chemical reactors.

The paper presents simulation experiments with the CSTR for hydrolysis of propylene oxide to propylene glycol. The reactor is exothermic one. There are two parameters with only approximately known values in the reactor. The steady state analysis shows that the reactor has multiple steady states and the open-loop analysis confirms that the reactor is open-loop unstable around one of these steady states. Then the possibility to stabilize the reactor using robust static output feedback PI and PID controllers is studied by simulations.

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MODEL OF THE CSTR

Hydrolysis of propylene oxide to propylene glycol in a continuous stirred tank reactor (Molnár et al., 2002) was chosen as a controlled process. The reaction is as follows

$$C_3H_6O + H_2O \longrightarrow C_3H_8O_2 \tag{1}$$

The reaction is of the first order with respect to propylene oxide as a key component. The dependence of the reaction rate constant on the temperature is described by the Arrhenius equation

$$k = k_{\infty} e^{-\frac{E_a}{RT_r}} \tag{2}$$

where k_{∞} is the pre-exponential factor, E_a is the activation energy, R is the universal gas constant and T_r is the temperature of the reaction mixture. Assuming ideal mixing in the reactor, the constant reaction volume and the same volumetric flow rates of the inlet and outlet streams, the mass balance for any component j in the system is

$$V_r \frac{dc_j}{dt} = q_r \left(c_{j0} - c_j \right) + \nu_j r V_r,$$
(3)

where V_r is the reaction volume, c is the molar concentration, q is the volumetric flow rate, ν is the stoichiometric coefficient, r is the molar rate of the chemical reaction and subscripts denote j the component, r the reation mixture, 0 the feed. It is assumed further that the specific heat capacities, densities and volumetric flow rates do not depend on temperature and composition, and also the heat of mixing and the mixing volume can be neglected. The simplified enthalpy balance of the reaction mixture used as a standard at reactor design (Ingham et al., 1994) is

$$V_r \rho_r C_{Pr} \frac{dT_r}{dt} = q_r \rho_r C_{Pr} \left(T_{r0} - T_r \right)$$
(4)
$$-UA \left(T_r - T_c \right) + r V_r \left(-\Delta_r H \right)^o$$

and the simplified enthalpy balance of the cooling medium is

$$V_c \rho_c C_{Pc} \frac{dT_c}{dt} = q_c \rho_c C_{Pc} \left(T_{c0} - T_c \right) + UA \left(T_r - T_c \right)$$
(5)

where T is the temperature, ρ is the density, C_P is the specific heat capacity, $(-\Delta_r H)^o$ is the reaction enthalpy, U is the overall heat transfer coefficient and A is the heat exchange area. The subscripts denote 0 the feed, c the cooling medium and r the reaction mixture. The values of constant parameters and steady-state inputs of the CSTR are summarized in Table 1.

Model uncertainties of the over described reactor follow from the fact that there are two physical parameters in this reactor, the reaction enthalpy and the preexponential factor, which values are known within following intervals (Table 2). The nominal values of these parameters are mean values of the intervals and they are

Table 1: Constant parameters and steady-state inputs of the CSTR

Variable	Value	Unit
V_r	2.407	m^3
V_c	2	m^3
$ ho_r$	947.19	${ m kg}~{ m m}^{-3}$
$ ho_c$	998	$\mathrm{kg}~\mathrm{m}^{-3}$
C_{Pr}	3.7187	$kJ kg^{-1}K^{-1}$
C_{Pc}	4.182	$kJ kg^{-1}K^{-1}$
AU	120	$kJ min^{-1}K^{-1}$
E_a/R	10183	Κ
q_r	0.072	$m^3 min^{-1}$
q_c	0.6307	${ m m}^3{ m min}^{-1}$
$c_{\mathrm{C_3H_6O},0}$	0.0824	$ m kmolm^{-3}$
$c_{\mathrm{C_3H_8O_2,0}}$	0	$ m kmolm^{-3}$
T_{r0}	299.05	Κ
T_{c0}	288.15	K

used for deriving of the nominal model of the CSTR. The minimal and maximal values of the intervals are used for obtaining models, which create the vertex systems (7).

Table 2: Uncertain parameters of the CSTR

Parameter	$(-\Delta_r H)^o$	k_{∞}
Unit	kJ kmol $^{-1}$	\min^{-1}
Minimal Value	-5.28×10^{6}	2.4067×10^{11}
Maximal Value	-5.64×10^{6}	3.2467×10^{11}

STEADY-STATE AND OPEN-LOOP ANALYSIS

The steady-state model of the CSTR in the form of a set of nonlinear algebraic equations (AEs) is obtained from the dynamic model (3) - (5) equating the derivative terms to zero. MATLAB function fsolve can be used for solving of the set of nonlinear AEs. The steady state behaviour of the chemical reactor with nominal values and also with 4 combinations of minimal and maximal values of 2 uncertain parameters was studied at first. It can be stated the reactor has always three steady states, two of them are stable and one is unstable. The situation is shown in Figure 1, where the curve Q_{GEN} (the curve is marked with * for the nominal model) represents the heat generated by the reaction and the line Q_{OUT} is the heat withdrawn from the reactor. The steady states of the reactor are points, where the curves and the line intersect. The steady states are stable if the slope of the cooling line is higher than the slope of the heat generated curve. This condition is satisfied for the nominal model at $T_r = 296.7$ K and $T_r = 377.5$ K, and is not satisfied at $T_r = 343.1$ K.

From the viewpoint of safety operation or in the case when the unstable steady-state coincides with the point that yields the maximum reaction rate at a prescribed temperature, it can be necessary to control a CSTR about its open-loop unstable steady-state, see e. g. (Pedersen and Jørgensen, 1999), (Antonelli and Astolfi, 2003),



Figure 1: Multiple steady states of the CSTR

(González and Alvarez, 2006).

In this context, the open-loop behaviour of the reactor in the surroundings of its unstable steady state at $T_r = 343.1$ K was studied at first. The initial temperature of the reaction mixture was chosen $T_r(0) = 346.95$ K. Simulation results obtained for the nominal model (curve with *) and 4 vertex systems are shown in Figures 2. They confirm that without feedback control, the temperature of the reaction mixture in the CSTR converges to the values characteristic either for the upper or the lower stable steady states.



Figure 2: Open-loop response of the CSTR

ROBUST STATIC OUTPUT FEEDBACK CONTROL

Consider a linear time-invariant system

$$\begin{aligned} \dot{\boldsymbol{x}}(t) &= \boldsymbol{A}\boldsymbol{x}(t) + \boldsymbol{B}\boldsymbol{u}(t), \quad \boldsymbol{x}(t_0) = \boldsymbol{x}_0 \\ \boldsymbol{y}(t) &= \boldsymbol{C}\boldsymbol{x}(t) \end{aligned}$$

where $\boldsymbol{x}(t) \in \mathbb{R}^n$ is the state, $\boldsymbol{u}(t) \in \mathbb{R}^m$ the control, $\boldsymbol{y}(t) \in \mathbb{R}^r$ the output, matrices $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$ have appropriate dimensions.

Consider further, the system (6) is a polytop of linear time-invariant systems

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{A}_{i}\boldsymbol{x}(t) + \boldsymbol{B}_{i}\boldsymbol{u}(t), \quad \boldsymbol{x}(t_{0}) = \boldsymbol{x}_{0}$$

$$\boldsymbol{y}(t) = \boldsymbol{C}_{i}\boldsymbol{x}(t)$$

$$i = 1, \dots, N$$

$$(7)$$

which represent vertices of (6) and matrices A, B, Care convex envelopes of matrices A_i, B_i, C_i , respectively, i = 1, ..., N. The number of vertex systems $N = 2^p$, where p is the number of uncertain parameters of (6).

Static Output Feedback With P Controller

Assume that it is necessary to find for the system (6) a static output feedback

$$\boldsymbol{u}(t) = \boldsymbol{F}\boldsymbol{y}(t) \tag{8}$$

with $\boldsymbol{F} \in \mathbb{R}^{m \times r}$ such that the closed loop system

$$\dot{\boldsymbol{x}}(t) = (\boldsymbol{A} + \boldsymbol{B}\boldsymbol{F}\boldsymbol{C})\,\boldsymbol{x}(t) = \boldsymbol{A}_{CL}\boldsymbol{x}(t) \qquad (9)$$

is stable, i.e. eigenvalues of A_{CL} have negative real parts. Finding of F is important when the state matrix A is unstable since having F leads to a stabilizing static output feedback.

But the output feedback (8) does not have integral action. One way of forcing an integral action to the output feedback is to put a set of integrators at the output of the plant, see e.g. Mikleš et al. (2006), Puna and Bakošová (2007). Forcing of derivative action to the output feedback has analogous basement.

Static output feedback with PI controller

For the system (6), it is necessary to find a static output feedback

$$\boldsymbol{u}(t) = \boldsymbol{F_1}\boldsymbol{y}(t) + \boldsymbol{F_2} \int_0^t \boldsymbol{y}(\tau) \mathrm{d}\tau \qquad (10)$$

with $F_1, F_2 \in \mathbb{R}^{m \times r}$.

Define a new state $\mathbf{z}(t) = [\mathbf{z}_1^T(t), z_2^T(t)]^T$, where $\mathbf{z}_1(t) = \mathbf{x}(t)$ and $\mathbf{z}_2(t) = \int_0^t \mathbf{y}(\tau) d\tau$. The dynamics of the newly defined system can be described as follows

$$\dot{\boldsymbol{z}}_{1}(t) = \dot{\boldsymbol{x}}(t) = \boldsymbol{A}\boldsymbol{z}_{1}(t) + \boldsymbol{B}\boldsymbol{u}(t), \ \boldsymbol{x}_{0} \quad (11)$$
$$\dot{\boldsymbol{z}}_{2}(t) = \boldsymbol{u}(t) = \boldsymbol{C}\boldsymbol{z}_{1}(t) \quad (12)$$

or

$$\dot{\boldsymbol{z}}(t) = \overline{\boldsymbol{A}}\boldsymbol{z}(t) + \overline{\boldsymbol{B}}\boldsymbol{u}(t),$$
 (13)

where

$$\overline{A} = \begin{pmatrix} A & 0 \\ C & 0 \end{pmatrix}, \overline{B} = \begin{pmatrix} B \\ 0 \end{pmatrix}.$$
 (14)

The output of the newly defined system is described as follows

$$\overline{\boldsymbol{y}}(t) = \overline{\boldsymbol{C}}\boldsymbol{z}(t),$$
 (15)

where

$$\overline{C} = \left(\begin{array}{cc} C & 0\\ 0 & I \end{array}\right) \tag{16}$$

with $\boldsymbol{I} \in \mathbb{R}^{r \times r}$.

So, the design of a static output feedback PI controller (10) can be transformed to the design of a static output feedback P controller

$$\boldsymbol{F} = \begin{bmatrix} \boldsymbol{F}_1 & \boldsymbol{F}_2 \end{bmatrix} \tag{17}$$

for the system (13) and (15).

Static output feedback with PID controller

For the system (6), it is necessary to find a static output feedback

$$\boldsymbol{u}(t) = \boldsymbol{F}_1 \boldsymbol{y}(t) + \boldsymbol{F}_2 \int_0^t \boldsymbol{y}(\tau) \mathrm{d}\tau + \boldsymbol{F}_3 \frac{\mathrm{d}\boldsymbol{y}(t)}{\mathrm{d}t} \quad (18)$$

with $\boldsymbol{F}_1, \boldsymbol{F}_2, \boldsymbol{F}_3 \in \mathbb{R}^{m \times r}$.

Define again a new state $\boldsymbol{z}(t) = [\boldsymbol{z}_1^T(t), \boldsymbol{z}_2^T(t)]^T$, where $\boldsymbol{z}_1(t) = \boldsymbol{x}(t)$ and $\boldsymbol{z}_2(t) = \int_0^t \boldsymbol{y}(\tau) d\tau$. Use $\boldsymbol{z}(t)$ and (6) leads to

$$\boldsymbol{y}(t) = \boldsymbol{C}\boldsymbol{z}_1(t) = \begin{pmatrix} \boldsymbol{C} & \boldsymbol{0} \end{pmatrix} \boldsymbol{z}(t)$$
 (19)

$$\int_{0}^{t} \boldsymbol{y}(t) dt = \boldsymbol{z}_{2}(t) = \begin{pmatrix} \boldsymbol{0} & \boldsymbol{I} \end{pmatrix} \boldsymbol{z}(t)$$
(20)

$$\frac{\mathrm{d}\boldsymbol{y}(t)}{\mathrm{d}t} = \boldsymbol{C}\dot{\boldsymbol{x}}(t) = \boldsymbol{C}\boldsymbol{A}\boldsymbol{x}(t) + \boldsymbol{C}\boldsymbol{B}\boldsymbol{u}(t) = \\ \begin{pmatrix} \boldsymbol{C}\boldsymbol{A} & \boldsymbol{0} \end{pmatrix} \boldsymbol{z}(t) + \boldsymbol{C}\boldsymbol{B}\boldsymbol{u}(t) \quad (21) \end{cases}$$

After the substitution (19), (20) and (21) into (18) and under the assumption that the matrix $F_4 = (I - F_3 CB)^{-1}$ exists, we obtain

$$\boldsymbol{u}(t) = \overline{\boldsymbol{F}}_1 \overline{\boldsymbol{y}}_1(t) + \overline{\boldsymbol{F}}_2 \overline{\boldsymbol{y}}_2(t) + \overline{\boldsymbol{F}}_3 \overline{\boldsymbol{y}}_3(t)$$
(22)

where $\overline{\boldsymbol{y}}_i(t) = \overline{\boldsymbol{C}}_i \boldsymbol{z}(t), i = 1, 2, 3, \overline{\boldsymbol{C}}_1 = (\underline{\boldsymbol{C}} \ \mathbf{0}),$ $\overline{\boldsymbol{C}}_2 = (\mathbf{0} \ \mathbf{I}), \overline{\boldsymbol{C}}_3 = (\mathbf{C} \mathbf{A} \ \mathbf{0}), \overline{\boldsymbol{F}}_1 = \boldsymbol{F}_4 \boldsymbol{F}_1, \overline{\boldsymbol{F}}_2 =$ $\boldsymbol{F}_4 \boldsymbol{F}_2$ and $\overline{\boldsymbol{F}}_3 = \boldsymbol{F}_4 \boldsymbol{F}_3$.

Defining

at

$$\overline{\boldsymbol{F}} = \left(\overline{\boldsymbol{F}}_1 \quad \overline{\boldsymbol{F}}_2 \quad \overline{\boldsymbol{F}}_3 \right), \qquad (23)$$

$$\overline{\boldsymbol{y}}(t) = \begin{pmatrix} \overline{\boldsymbol{y}}_1^T(t) & \overline{\boldsymbol{y}}_2^T(t) & \overline{\boldsymbol{y}}_3^T(t) \end{pmatrix}^T, \quad (24)$$

$$\overline{C} = \left(\overline{C}_1^T \quad \overline{C}_2^T \quad \overline{C}_3^T \right)^{\prime}, \qquad (25)$$

we obtain a new dynamic system

$$\dot{\boldsymbol{z}}(t) = \overline{\boldsymbol{A}}\boldsymbol{z}(t) + \overline{\boldsymbol{B}}\boldsymbol{u}(t)$$

$$\overline{\boldsymbol{y}}(t) = \overline{\boldsymbol{C}}\boldsymbol{z}(t)$$
(26)

with

$$\boldsymbol{u}(t) = \overline{\boldsymbol{F}}\overline{\boldsymbol{y}}(t)$$
 (27)

and

$$\overline{A}=\left(egin{array}{cc} A & 0 \ C & 0 \end{array}
ight), \overline{B}=\left(egin{array}{cc} B \ 0 \end{array}
ight), \overline{C}=\left(egin{array}{cc} C & 0 \ 0 & I \ CA & 0 \end{array}
ight)$$

So, the design of a static output feedback PID controller is transformed to the design of a static output feedback P controller for the system (26). After finding the P controller $\overline{F} = (\overline{F}_1 \ \overline{F}_2 \ \overline{F}_3)$, we obtain the PID controller

$$\boldsymbol{F} = \begin{bmatrix} \boldsymbol{F}_1 & \boldsymbol{F}_2 & \boldsymbol{F}_3 \end{bmatrix}$$
(28)

as follows

$$\boldsymbol{F}_3 = \boldsymbol{\overline{F}}_3 (\boldsymbol{I} + \boldsymbol{C} \boldsymbol{B} \boldsymbol{\overline{F}}_3)^{-1}$$
(29)

$$\boldsymbol{F}_2 = (\boldsymbol{I} - \boldsymbol{F}_3 \boldsymbol{C} \boldsymbol{B}) \boldsymbol{F}_2 \tag{30}$$

$$\boldsymbol{F}_1 = (\boldsymbol{I} - \boldsymbol{F}_3 \boldsymbol{C} \boldsymbol{B}) \boldsymbol{F}_1 \tag{31}$$

Robust static output feedback controller design

Consider an uncertain polytopic closed-loop system with the system (6) and one of static output feedback controllers (8), (17) and (28). The closed-loop system is described

$$\dot{\boldsymbol{x}}(t) = [\boldsymbol{A} + \boldsymbol{B}\boldsymbol{F}\boldsymbol{C}]\,\boldsymbol{x}(t) = \boldsymbol{A}_{CL}\boldsymbol{x}(t) \qquad (32)$$

where A_{CL} is a convex envelope of a set of linear time invariant matrices A_{CLi}

$$\boldsymbol{A}_{CLi} = \boldsymbol{A}_i + \boldsymbol{B}_i \boldsymbol{F} \boldsymbol{C}_i, \ i = 1, \dots, N$$
(33)

System (32) is quadratically stable if and only if there exists a positive definite matrix P > 0 such that following inequalities hold

$$\boldsymbol{A}_{CLi}^{T}\boldsymbol{P} + \boldsymbol{P}\boldsymbol{A}_{CLi} < 0, \ \boldsymbol{P} > 0, \ i = 1, \dots, n \quad (34)$$

Consider the uncertain polytopic system (6). Two following statements are equivalent according to Veselý (2002).

1. The system (32) is simultaneously static output feedback stabilizable with guaranteed cost J^*

$$\int_{0}^{\infty} \left[\boldsymbol{x}(t)^{T} \boldsymbol{Q} \boldsymbol{x}(t) + \boldsymbol{u}(t)^{T} \boldsymbol{R} \boldsymbol{u}(t) \right] dt \leq \boldsymbol{x}_{0}^{T} \boldsymbol{P} \boldsymbol{x}_{0} = J^{*}, \ \boldsymbol{P} > 0$$
(35)

2. There exist matrices P > 0, Q > 0, R > 0 and a matrix F such that the following inequalities hold

$$\boldsymbol{A}_{i}^{T}\boldsymbol{P} + \boldsymbol{P}\boldsymbol{A}_{i} - \boldsymbol{P}\boldsymbol{B}_{i}\boldsymbol{R}^{-1}\boldsymbol{B}_{i}^{T}\boldsymbol{P} \\ + \boldsymbol{Q} \leq 0, \quad i = 1, \dots, n \quad (36) \\ (\boldsymbol{B}_{i}^{T}\boldsymbol{P} + \boldsymbol{R}\boldsymbol{F}\boldsymbol{C}_{i})\boldsymbol{\phi}_{i}^{-1}(\boldsymbol{B}_{i}^{T}\boldsymbol{P} + \boldsymbol{R}\boldsymbol{F}\boldsymbol{C}_{i})^{T} \\ - \boldsymbol{R} \leq 0, \quad i = 1, \dots, n \quad (37) \end{cases}$$

where

$$\phi_i = - (A_i^T P + P A_i - P B_i R^{-1} B_i^T P + Q), \quad i = 1, \dots, n$$
(38)

The second statement is used for the design of a static feedback controller for simultaneous stabilization of the system (32) with guaranteed cost (35) (Veselý, 2002). Using the Schur complement and defining $S = P^{-1}$, the inequality (36) is transformed to the following LMIs

$$\begin{bmatrix} \boldsymbol{S}\boldsymbol{A}_{i}^{T} + \boldsymbol{A}_{i}\boldsymbol{S} - \boldsymbol{B}_{i}\boldsymbol{R}^{-1}\boldsymbol{B}_{i}^{T} & \boldsymbol{S}\sqrt{\boldsymbol{Q}} \\ \sqrt{\boldsymbol{Q}}\boldsymbol{S} & -\boldsymbol{I} \end{bmatrix} \leq 0$$

$$\gamma\boldsymbol{I} < \boldsymbol{S}, \quad i = 1, \dots, n \qquad (39)$$

where $\gamma > 0$ is any non-negative constant.

Using $P = S^{-1}$, the inequality (37) can be rewritten to the following LMIs

$$\begin{bmatrix} -\boldsymbol{R} & \boldsymbol{B}_i^T \boldsymbol{P} + \boldsymbol{R} \boldsymbol{F} \boldsymbol{C}_i \\ (\boldsymbol{B}_i^T \boldsymbol{P} + \boldsymbol{R} \boldsymbol{F} \boldsymbol{C}_i)^T & -\boldsymbol{\phi}_i \end{bmatrix} \leq 0$$
$$i = 1, \dots, n \qquad (40)$$

The algorithm has following steps.

- 1. Compute $\boldsymbol{S} = \boldsymbol{S}^T > 0$ from the LMIs (39).
- 2. $P = S^{-1}$.
- 3. Compute F from the LMIs (40).
- 4. If the solution of (39) is not feasible, the system (32) is not simultaneously stabilizable by a static output feedback. If the solution of (40) is not feasible, the closed-loop system (32) is not quadratically stable with guaranteed cost. Then change Q, R or γ in order to find feasible solutions.

There are two parameters in the presented algorithm, which can be called tuning parameters. They are weighting matrices Q and R in (35). The choice of γ in (39) also influences the solution, but γ is only a LMI variable.

ROBUST STABILIZATION OF THE CSTR

The main aim was to study possibility to stabilize the described CSTR around the open-loop unstable steady state at the temperature $T_r = 343.1$ K using static output feedback PI and PID controllers.

It was necessary to obtain a linear state space model (6) of the controlled process at first. The model was derived using linearization of non-linear terms in the mathematical model (3)–(5). The working point for linearization was the unstable steady state. It was supposed for control purposes that the reactor was the two-input single-output system. The reaction mixture flow rate q_r and the coolant flow rate q_c were chosen as the control inputs and the temperature of the reaction mixture T_r was selected as the controlled output. For 2 uncertain parameters, we obtained one nominal system and $2^2 = 4$ vertex systems (7). All these systems were unstable.

For finding stabilizing output feedback PI or PID controllers, it was necessary to solve two sets of LMIs (39), (40), each set consisting of 4 LMIs. The feasibility of the solution of (39) assured that the reactor was robust static output feedback quadratically stabilizable and the feasibility of the solution of (40) gave robust static output stabilizing controller with guaranteed cost for the whole uncertain system. For solving of LMIs, the LMI MATLAB Toolbox was used. Following parameters influenced solution and could be changed: Q, R, γ . In dependence on the choice of these parameters, it was possible to find several stabilizing PI and PID controllers. Two of them are presented in Table 3 and they were obtained with

Values of elements of Q and R were chosen with respect to the values of state and input variables.

Table 3: Stabilizing PI and PID controllers

	PI	PID
F_1	$\left[\begin{array}{c} 3.08 \times 10^{-2} \\ 5.43 \times 10^{-1} \end{array}\right]$	$\left[\begin{array}{c}9.71\times10^{-2}\\4.89\end{array}\right]$
F_2	$\left[\begin{array}{c} 8.51 \times 10^{-3} \\ 2.24 \times 10^{-1} \end{array}\right]$	$\left[\begin{array}{c} 3.53 \times 10^{-2} \\ 1.83 \end{array}\right]$
F_3		$\left[\begin{array}{c} 1.43 \times 10^{-2} \\ 3.65 \end{array}\right]$

The possibility to stabilize the reactor using designed robust static output feedback PI and PID controllers was studied by simulations. The nonlinear model of the CSTR was used as the controlled system and the initial temperature of the reaction mixture was $T_r(0) =$ 346.95 K. The aim was to control the temperature in the CSTR about the value $T_r = 343.1$ K. The control input boundaries were as follows: $q_r \in [0; 0.18]$ m³min⁻¹ and $q_c \in [0; 1.58] \text{ m}^3 \text{min}^{-1}$. Following disturbances in the feed temperature of the reaction mixture were loaded: T_{r0} increased by 4 K for $t \in [20; 70)$ min and decreased by 8 K for $t \in [70; 100)$ min. Obtained simulation results are shown in Figures 3, 4. Both, PI and PID static output feedback controllers are able to stabilize the CSTR with uncertainties about its open-loop unstable steady state. The robust PID controller attenuates disturbances very fast and the overshoots caused by disturbances are minimal.



Figure 3: Robust PI stabilization of the CSTR - controlled output

In praxis, it is necessary to work with noisy signals. The ability of robust static output feedback PI a PID controllers to stabilize the CSTR with noisy signals was studied, too. The white noise with noise power 0.0005 was added to the controlled output. The load disturbances were the same as in the previous case. Obtained simulation results are shown in Figures 5 - 10. Robust PI and PID controllers are able to stabilize the CSTR with noisy signals, but PID controllers can generate control inputs which cannot be realized.



Figure 4: Robust PID stabilization of a CSTR - controlled output

CONCLUSION

In this paper, the possibility to use simulations for steadystate, open-loop and closed-loop analysis of the CSTR for hydrolysis of propylene oxide to propylene glycol was studied. The main aim was to study the possibility to stabilize the exothermic CSTR with uncertain parameters using static output feedback PI and PID controllers. The non-iterative algorithm for design of robust static output feedback PID like controllers is presented. The design of robust controllers is based on solution of LMI, for which the MATLAB LMI Toolbox can be succesfully used. Simulations confirmed that robust static output feedback PI or PID controllers can be successfully used for control of CSTRs with multiple steady states, uncertainties and disturbances, even though CSTRs are very complicated systems from the control point of view. The advantage of robust PI and PID controllers is that they do not retain steady-state control errors and they both are are able stabilize the open-loop unstable processes. All simulations were done using MATLAB 6.5.

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Figure 5: Robust PI stabilization of the CSTR with disturbances and noisy signals - controlled output



Figure 6: Robust PI stabilization of the CSTR with disturbances and noisy signals - control input q_r



Figure 7: Robust PI stabilization of the CSTR with disturbances and noisy signals - control input q_c



Figure 8: Robust PID stabilization of the CSTR with distubances and noisy signals - controlled output



Figure 9: Robust PID stabilization of the CSTR with distubances and noisy signals - control input q_r



Figure 10: Robust PID stabilization of the CSTR with distubances and noisy signals - control input q_c

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ELMAN NEURAL NETWORKS IN MODEL PREDICTIVE CONTROL

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KEYWORDS

Model predictive control, Elman neural network, predictor

ABSTRACT

The goal of this paper is to present interesting way how to model and predict nonlinear systems using recurrent neural network. This type of artificial neural networks is underestimated and marginalized. Nevertheless, it offers superior modelling features at reasonable computational costs. This contribution is focused on Elman Neural Network, two-layered recurrent neural network. The abilities of this network are presented in the nonlinear system control. The task of the controller is to control the liquid level in the second of two interconnected cylindrical tanks. The mathematical model of the realtime system was derived in order to test predictor and consequently the controller in Matlab/Simulink simulations.

INTRODUCTION

Model predictive control (MPC) (Camacho and Bordons 2007) is a very popular concept for the development and tuning of nonlinear controllers in the presence of input, output or state constraints. Many predictive control techniques based on MPC that use artificial neural network (ANN) as a predictor are established on multilayer feed-forward neural networks (Hagan et al. 2002), (Kanjilal 1995). In spite the multilayer feedforward neural networks (MFFNNs) have many advantages such as simple design and scalability, they have also many drawbacks such as long training times and choice of an appropriate learning stop time (the over-learning versus the early stopping problem). However, there is quite a number of types ANNs suitable for the modelling and prediction, for instance adaptive linear networks, radial basis function networks and recurrent networks (Liu 2001), (Meszaros et al. 1999), (Koker 2006).

This paper is divided as follows: After short introduction to the recurrent neural networks, the used model predictive controller is explained. Then the model of the real time system is derived. After that the identification of the predictor (training of the artificial neural network) is described. When the identification is finished, the paper focuses on the model predictive control and evaluation of results. The contribution is finished by some concluding remarks.

RECURRENT NEURAL NETWORKS

Recurrent neural networks (sometimes are these networks called feedback neural networks) can be distinguished from feed-forward neural networks in that they have a loopback connection (Figure 1). In its most general form recurrent network consist of a set of processing units, while the output of each unit is fed as input to all other units including the same unit. With each link connecting any two units, a weight is associated which determines the amount of output a unit feeds as input to the other unit (Yegnanarayana 2005).



Figure 1: Example of Recurrent Neural Network

Recurrent neural networks have superior temporal and spatial behaviours, such as stable and unstable fixed points and limit cycles, and chaotic behaviours. These behaviours can be utilized to model certain cognitive functions, such as associative memory, unsupervised learning, self-organizing maps, and temporal reasoning (He 1999).

Elman Neural Networks

One of the most known recurrent neural networks is Elman neural network (Elman 1990). Typical Elman network has one hidden layer with delayed feedback. The Elman neural network is capable of providing the standard state-space representation for dynamic systems. This is the reason why this network architecture is utilized as a recurrent neural equalizer.

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) Generally, this network is considered as a special kind feed-forward network, including additional memory neurons and local feedback (Koker 2006). Typical structure of Elman neural network is depicted in fig. 2.



Figure 2: Elman Neural Network

MODEL PREDICTIVE CONTROL

There are various approaches to predictive control by artificial neural networks. Generally we can say that these methods use ANN as the plant model in order to get its output predictions. The most used approach is model predictive control (Camacho and Bordons 1995). MPC is a broad control strategy applicable to both linear and nonlinear processes.

The main idea of MPC algorithms is to use a dynamical model of process to predict the effect of future control actions on the output of the process. Hence, the controller calculates the control input that will optimize the performance criterion over a specified future time horizon:

$$J = \lambda \cdot \sum_{i=N_1}^{N_2} [w(k+i) - \hat{y}(k+i)]^2 + \rho \cdot \sum_{i=1}^{N_u} [u_i(k+i-1) - u_i(k+i-2)]^2$$
(1)

where N_1 , N_2 and N_u define horizons over which the tracking error and the control increments are evaluated (usually $N_2 \ge N_u$). The u_t variable is the tentative control signal, w is the desired response and \hat{y} is the network model response. The parameters λ and ρ determine the contribution that the sums of the squares of the future control errors and control increments have on the performance index.

There is usually assumed that after a certain interval N_u < N_2 there is no variation in the proposed control signals, that is:

$$\Delta u(k+i) = 0 \text{ for } i \in \langle N_u, N_2 - 1 \rangle$$
 (2)

This is equivalent to giving infinite weights to the changes in the control from a certain instant. This approach is adopted in this paper.

SIMULATIONS

In this chapter, the mathematical model of the real time system is derived first. Then the identification of the predictor is presented. After that the MPC controller is used in Matlab/Simulink for control of nonlinear system.

Modelling the Real-time System

Let us consider SISO nonlinear system to be controlled which is shown in the figure 3 and consist two connected cylindrical tanks for liquid. The dynamic model if the system is (considering usual simplifications):

$$q_{1v} = q_1 + \frac{\pi d_1^2}{4} \cdot \frac{dh_1}{dt}$$
(3)

$$q_1 = q_2 + \frac{\pi d_2^2}{4} \cdot \frac{dh_2}{dt}$$
 (4)

$$q_1 = k_1 \sqrt{h_1 - h_2}$$
 (5)

$$q_2 = k_2 \sqrt{h_2} \tag{6}$$

where d_j is the diameter, h_j is liquid level and q_j is the output flow of the *j*-th tank. $q_{1\nu}$ is the input flow to the first tank. The constants associated with the properties of pipes and valves are k_1 and k_2 . The objective of the controller is to maintain the level in the second tank h_2 (output value) by adjusting the input flow $q_{1\nu}$ (control signal).



Figure 3: Scheme of Two Interconnected Cylindrical Tanks

This system is based on real-time laboratory model Amira DTS-200 (figure 4) which consist 3 cylindrical tanks and two pumps. However, in this contribution only two tanks (T1 and T2) and one pump were selected. Thus, the valves V2 and V4 were fully closed and the valve number 5 was set to the half position.

The values of parameters are $k_1=11.53 \text{ cm}^{2.5}/\text{s}$ and $k_2 = 13.09 \text{ cm}^{2.5}/\text{s}$ were obtained by experiments on the DTS-200. The maximum input flow $q_{1\nu}$ is 100 cm³/s. The height of the tanks is 60 cm and their diameter is 14 cm.



Figure 4: Scheme of Amira DTS-200

The mathematical model was transformed into the Simulink as is depicted in the figure 5. The Simulink model is more general and consist possibility to model TITO (two inputs – two outputs) system with two pumps and observation of level of liquid in both tanks.



Figure 5: Simulink Model of the Two Cylindrical Tanks System

Predictor Based on Elman Neural Network

As was mentioned hereinbefore, in this paper Elman Neural Network was used as a predictor of the controlled system. The structure follows figure 2. The predictor consisted of five neurons with hyperbolic tangent transfer function in hidden layer and one neuron with linear transfer function in the output layer.

In this chapter two variants of predictor are introduced. The first one used five last values of control signal and output signal, thus it had ten inputs. This predictor is further referred to as *predictor1*. The second predictor utilized only five past values of the output signal. This predictor is further referred to as *predictor2*.

Both predictors were trained offline for identification data obtained using stepped actuating signal. For the off-line identification was used input-output data generated by pulses of random amplitude and duration. Duration and amplitude of the pulses must be chosen carefully to produce accurate identification. The amplitudes in range <0; 100> cm3/s and duration from 1s to 50s were used. The Levenberg-Marquardt

backpropagation algorithm implemented in the Matlab Neural Network Toolbox was applied as training function. Final predictors were tested on the training data (figures 6 and 8) and unknown testing data as well (figures 7 and 9).



Figure 6: Training Data Response of predictor1



Figure 7: Testing Data Response of predictor1



Figure 8: Training Data Response of predictor2

As can be seen from figures, *predictor1* suffers from a disturbance. This is caused by step-shaped identification control signal. Each of steep bounce of predicted signal is caused by steep step change of control signal at the predictor input. This behaviour can be easily removed by omitting the control signal at the predictor 2). Difference between both predictors is shown in the Table 1, where are presented mean square prediction error (MSPE) values for from 1 to 5-step ahead predictions of the same testing data.



Figure 9: Testing Data Response of predictor2

Table 1: Mean Square Prediction Errors – Comparison of the Predictors

	MSPE				
	1 step	2 step	3 step	4 step	5 step
predictor1	2,79	5,89	9,11	13,51	18,66
predictor2	0,86	1,72	2,81	4,92	6,95

Control of Two Connected Cylindrical Tanks

Simulations were done for both predictors. As can be seen from figure 10 the control loop was simulated in Matlab/Simulink. The sampling period of Simulink was set to 1s. Because the SISO system is regarded, the input flow to the second tank is set to zero and the level of liquid in the first tank is not used.



Figure 10: Simulink Scheme of the Control Loop

Due to constraints and nonlinear nature of predictors numerical optimization of the MPC criterion was necessary. The controller used constrained quasi-Newton method from Matlab Optimization Toolbox as a nonlinear optimization algorithm.

TDL blocks in the figure 10 represents so called Tapped Delay Line which stores five recent values of the signals. This block is necessary because artificial neural network uses five recent values of system input and output. Structure of TDL for is depicted in figure 11.



Figure 11: TDL Block from the Simulink Control Loop

A vast number of simulations were done due to find optimal setting of the controller. From comparability reasons the same controller settings is used for the both predictors: $\lambda = 1$, $\rho = 0.001$, $N_1 = 1$, $N_2 = 5$, $N_u = 5$. Simulations results are presented in figures 12 and 13.



Figure 12: Control using predictor1

In order to compare results of both controllers (predictors) we used two quadratic criterions:

$$S_{y} = \sum_{k} (w_{k} - y_{k})^{2}$$
(7)

$$S_{u} = \sum_{k} (u_{k} - u_{k-1})^{2}$$
(8)

The first criterion S_y is based on control errors and represents the tracking performance of the controller. While the second criterion S_u is based on changes of the control signal and represents the controller demands on the actuators. The computed values of both criterions are shown in the table 2.



Figure 13: Control using *predictor2*

 Table 2: Comparison of the Controllers/Predictors

 Using the Quadratic Criterions

Predictor Used	Quadratic Criterions	
in the Controller	$S_v [cm^2]$	$S_u [\mathrm{cm}^4/\mathrm{s}^2]$
predictor l	$1,27 \cdot 10^5$	112,08
predictor2	$1,18 \cdot 10^5$	1,31

CONCLUSIONS

As can be seen simulations, the usage of Elman neural networks as a predictor in model predictive control is possible, while special attention should be paid to modelling stage. The quality of predictor and its predictions is influenced by its structure and identification data.

The badly identified predictor (*predictor1*) didn't perform well in prediction task. However, it is worth noticing that model predictive controller is quite tolerant to a predictor inaccuracy, because (as can be seen from figure 12) the system output still tracks the reference.

The most significant aspect of this paper is the reduction in computational time. The model predictive control method involves highly mathematical computations. What is more, predictors based on artificial neural networks significantly increase computational demands of the MPC controllers. Nevertheless, Elman neural network provides very interesting way how to reduce computational costs, because the training times of Elman networks are incredibly short. This kind of artificial neural network could be promising for on-line adaption of the predictor in case of t-variant systems. This will be subject of further research.

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Simulation, Experimental Science and Engineering

DYNAMIC INTERACTION BETWEEN HEAVY VEHICLES AND SPEED BUMPS

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KEYWORDS

Computer simulation, heavy vehicles, speed bumps, LS-DYNA.

ABSTRACT

The paper presents finite element (FE) model development and experimental validation for a truck tractor with a three axle single drop lowboy trailer. The main objective of this research activity was to create a simplified, three dimensional virtual FE model, applicable for computer simulation of dynamic interaction between a vehicle and a bridge or road structure. Such model should provide a reliable approximation of dynamic loadings exerted by the wheels to the bridge or pavement structure for a wide range of total weights and speeds considered. To meet this requirement the FE model should have correct mass and properly represented stiffness distribution characteristics of the suspension system. As explicit laboratory testing of the suspension system requires its disassembling and is very expensive, an indirect method was applied to find the stiffness and damping characteristics of the suspension.

The study reported in this paper consists of experimental and numerical parts. During the experimental tests the vehicle was driven across the speed bumps at different speeds. The relative displacement and acceleration histories were recorded for several points located on the vehicle axles and the frame. In addition, a speed bump was scanned on site using a laser scanner. The experimental data was subsequently used for the development and calibration of the spring and damping characteristics for suspension systems of the FE model. The numerical part was based on non-linear, explicit, dynamic, finite element (FE) analysis using the LS-DYNA computer code.

INTRODUCTION

One of the important issues for maintenance and design engineers is the magnitude of actual dynamic loads exerted by heavy vehicles on bridges and roads. Experimental, analytical, and numerical studies were conducted to estimate the actual values of impact factors which represent dynamic overloading as compared with static loads (Kwasniewski et al. 2006). A need for consideration of a wide variety of heavy vehicle configurations suggests a selection of computer methods as the most effective and flexible. Heavy vehicles are usually considered in such analyses as simplified systems of rigid masses connected through linear or nonlinear springs and dampers (Fafard and Bennur 1997, Green and Cebon 1997, Huang et al. 1998, and Piombo et al. 2000). Besides the correct mass distribution, a model of a heavy vehicle should have an appropriate representation of the actual suspension system.

Characteristics of the vehicle suspension can be determined through experimental compression tests conducted either on an isolated suspension system or indirectly through field experiments conducted on an entire vehicle. The purpose of each test is to determine stiffness and damping characteristics of the suspension. The first method is expensive as it requires removal of the suspension from the existing vehicle or a purchase of a new one. Displacement of the piston of the shock absorber is measured and recorded as a function of the load applied. This relationship is non-linear and is usually simplified by piecewise linear functions. Idealized, perfectly fixed boundary conditions in direct suspension testing do not account for sometimes worn out and partially loose connections between the suspension and the vehicle. In addition, testing of a new suspension system will often result in different suspension characteristics as compared with those in actual and used vehicles.

In the indirect method the tests are conducted on an entire vehicle which moves along predefined road surface profiles with different loads and at different speeds (Lehtonen 2005, Letherwood and Gunter 2001, and Valášek et al. 1998). Typical data acquisition from such tests usually includes time histories of accelerations and relative displacements between selected points. Filtered experimental output is analyzed and used for validation of analytical or numerical models. The first approximation of the suspension characteristics can also be obtained for some of the technical solutions using simplified formula developed by the automotive industry. Such formula allow for calculation of linear stiffness of leaf spring suspension based on dimensions of leaves and their number. The disadvantage of the indirect method is the difficulty in measuring dynamic interaction forces between suspension components or between wheels and the road surface.

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Correct representation of wheel and tire models is another important issue in modeling of heavy vehicle dynamic behavior. In very simple models the wheels are represented by lumped masses with time dependent, moving, concentrated reactions. However, modern computational techniques allow modeling the wheels as rotating, pneumatic, three dimensional objects interacting with the road surface through a well defined contact algorithm. The burden of complexity of such an approach is addressed by the FE code used for the simulation. This type of approach is easier and more reliable as it requires fewer simplifying assumptions.

The main objective of this research activity is to develop a simplified FE model of a heavy vehicle applicable for transient analysis of dynamic interaction between a vehicle and a bridge or a road surface. Such a model provides a reliable approximation of dynamic loading exerted by the wheels on the bridge or pavement. It is expected that the procedure developed here will be easily adaptable for a wide range of heavy vehicles with different gross vehicle weights (GVW), suspension characteristics, and speeds. A popular heavy vehicle, a single unit tractor-trailer with a three axle single-drop lowboy, was chosen as representative for this study. The paper describes its FE model development and experimental validation through onsite experimental tests. A numerical analysis presented here is based on non-linear, explicit, dynamic, finite element (FE) computational mechanics using the LS-DYNA computer code. During the experimental tests the heavy vehicle was driven across a speed bump at different speeds. Relative displacement and acceleration histories were collected for several points located on vehicle's axles and frame. In addition, an actual, typical speed bump was scanned using a laser scanner and a resulting FE model of the speed bump was developed. The experimental data was subsequently used for the development and validation of the spring and damping characteristics for all suspension systems of the FE model.

FINITE ELEMENT MODELS

FE models of the Truck Tractor and Single-Drop Lowboy Trailer

The truck tractor, with a three axle single-drop lowboy trailer as shown in Figure 1a, was selected for this study. A complete FE model of the tractor and the trailer consists of over 25,000 finite elements. It is presented in Figure 1b with an additional cargo of the total mass of 39,000 kg. It is planned that this fully loaded vehicle will be used in further experimental tests of dynamic interaction between a bridge and a moving vehicle.

The HyperMesh Software from Altair was used as a preprocessor for modeling. In-situ measurements and data available from the manufacturers' websites were used for developing the FE model.

The selected truck is one of the most popular in the U.S. The wheelbase for the truck is 4.73 meters long and may vary between 3.68 and 6.10 meters. The tandem axle spacing in the rear suspension remains the same for each wheelbase. Therefore, future, simple modifications of the wheelbase in the FE model are possible and they can be easily implemented by adding or removing FE elements from the longitudinal truck frame.

Development of the suspension system and identification of its major components are presented in Figure 2. Each suspension consists of the rotating horizontal axles located along corresponding non-rotating axles which are connected to the frame through vertical cylindrical joints. All axles are modeled using rigid beam elements. The rotation of a rotating axle is implemented by using a constraint option, referred to as a revolute joint in LS-DYNA (LS-DYNA 2007).

The vertical movement of an axle set is achieved by using the cylindrical joints and the special purpose massless discrete elements which simulate springs and shock absorbers, as presented in Figure 2.



Figure 1: Selected Truck Tractor and Single-Drop Lowboy Trailer (a) and Their FE Model (b)





The entire FE model of the front suspension includes the steering axle, two leaf springs, and two shock absorbers. Other components such as the frame hangers, bushings, height control system, upper shock brackets and axle attachment hardware were lumped together as a sprung mass connected with the bodywork. Their mass was added to the equivalent parts connected with the frame through the Vertical Cylindrical Joint (see Figure 2). Tandem axles with air springs are modeled in the rear suspension system in the similar way as observed in the actual truck. Each axle suspension includes air springs, shock absorbers, a cross channel, main support members, an ultra rod, torque rods, an axle, and frame brackets. The total mass of these components was lumped together into an equivalent part in the FE model. In the suspension system of the actual trailer, two leaf springs per axle are used in an underslung configuration with a 127 mm round axle. The total weight of each suspension system was estimated based on the available data. In the FE model, the mass of each axle was distributed between rotating and non-rotating axles represented by 2D beam elements.

The actual truck has 22.5"×8.25" aluminum wheels, whereas the trailer is equipped with steel 2 hand-hole wheels 22.5"×7.50" in size. Two types of shell elements were used for modeling – 3-node elements for the discs and 4-node elements for the rims, see Figure 3. Both units have tubeless tires. A simple pressure volume airbag model was used for the FE pneumatic models of the tires. The values of pressure inside the airbags were set up according to data provided by the tire manufacturer and can be easily changed in the FE model. The FE model of the tire consists of the sidewalls and the tread parts. Each of these components includes two coincident layers of 4-node shell elements. The first layer represents rubber-like material with average properties for rubber, whereas the second layer (representing the cord) uses a material model for fabrics, with stiffness for tension only.

The thicknesses of the shell elements used for wheels and tires was based on the data available from manufacturer websites; however some of them were modified in order to obtain masses similar to the actual wheels. The FE model of the complete wheel including disc, rim, sidewalls, and tread, is presented in Figure 3.



Figure 3: FE Model of Wheel (a) and its Components – Sidewalls and Tread include Two Layers of Elements for Rubber and Fabric Materials

The major objective of this project was to determine the effect of the speed bumps on the dynamic behavior of the heavy vehicle. Therefore, the complete FE model of the tractor and trailer was simplified, as detailed modeling of each component was not necessary to achieve the project goal. The simplifications included primarily the bodywork where the driver cab, hood, fuel tanks, and engine were modeled as rigid bodies. Moreover, the FE models of the drive and steering systems were also simplified and they do not include transmission, transmission shafts and a few other components. These simplifications not only helped in reducing the size of the FE model and the CPU time needed but they also made all the calculations more stable and reliable.

The selected single drop lowboy trailer was constructed using standard U.S. structural steel profiles including: C-channels, S-flanges and wide flanges (Engineers Edge 2008). 4-node shell elements were used for the FE modeling. Additional load in the form of crane counterweights was modeled as a rigid body using solid elements.

The revolute joints were also used in the "fifth" wheel connection, as shown in Figure 4. They allow for the relative movement of the trailer in the vertical plane. For all of the performed analysis the FE model was restricted to the straight direction and any movements of the trailer in the horizontal plane were not allowed. Hence, the fifth wheel and the skid plate of the trailer were rigidly connected.

The suspension systems and the tires received much attention in the modeling process as clearly having a distinct influence on the interaction between vehicle and the road surface. Finding all the necessary data for suspension development took a significant amount of



Figure 4: FE Model of the Fifth Wheel (a). Connection between Fifth Wheel and the Skid Plate (b)

time during this project. The tires were modeled using elastic material that allows for large deformation, whereas the spring and damping elements of suspension systems were simplified by discrete elements with appropriate material properties. Such modeling strategy resulted in simplifications in the FE model, as well as a reduction in the total number of elements and CPU time.

The FE model validation began with checking mass distribution for each unit. In the corresponding FE analysis six rigid surfaces were placed under the vehicle wheels to simulate scales - one surface per axle. These surfaces were defined as *Rigidwall Planar Surfaces*. The complete FE model was dropped on the rigid surfaces under gravity and the load induced on each axle was registered. The vibrations caused by gravity application were damped using global external viscous damping. The data obtained were filtered using a cosine filter. At the beginning, the total calculated mass of the FE model was smaller than the weight of the actual vehicles due to the assumed simplifications mentioned above. Therefore, some modifications of material densities for a few selected components were made to obtain the appropriate mass distribution related to the values from experimental tests.

Table 1 shows the comparison of masses corresponding to the axle loads from the FE analysis and the measurements for the unloaded vehicle.

Table 1: Comparison of the Axle Loads from the FE Analysis and Measurements for the Unloaded Vehicle

	Axle Load	
Axle Type	Measurement	FE Analysis
	(kg)	(kg)
Front Steer	3,955	3,955
Forward Tandem Drive	2,676	2,677
Rear Tandem	3,012	3,015
First Trailer	3,021	3,025
Second Trailer	3,447	3,445
Third Trailer	3,946	3,943
TOTAL	20,057	20,060

FE Model of the Speed Bump

A laser scanner was used to capture geometry of actual speed bumps used in on-site experiments. This technique was used to develop FE models of the speed bumps for subsequent FE analyses. In the first step, the number of points obtained from the scanner was limited to those surrounding each speed bump. The scanned and selected points are shown in Figure 5a. The next step was to generate polynomial curves, based on the selected points, which were subsequently used to create surfaces. Finally, the surfaces were meshed using 4-node shell elements resulting in the FE model of the speed bump. Rigid material was applied for the speed bump elements due to their high stiffness as compared with the tires. The methodology of data processing for the cloud of points is depicted in Figure 5. A simple surface to surface contact model between bumps and tire models was used with a friction coefficient f = 0.65 (Engineer's Handbook 2008). All tire treads were included in the slave segment whereas the FE model of the speed bump was considered as the master in the tire and road surface contact model.





EXPERIMENTAL TESTING FOR SUSPENSION VALIDATION

Several preliminary tests were conducted to provide approximate data on spring stiffness and damping coefficients implemented in the FE model. These tests were carried out for the front (axle No. 1) and rear (axle No. 2 and 3) suspension systems of the truck, and for the trailer suspension system (axle No. 4, 5 and 6). During the tests the vehicle was dropped off a 75 mm high wooden plank placed under the wheels, as shown in Figure 6a. The vertical change in distance between the frame and the axle was measured using a linear displacement sensor. In addition, accelerations at the
axles and bodywork were registered. Two types of uniaxial accelerometers with a measurement range of $\pm 5g$ and $\pm 10g$ were used during the tests. The accelerometers with the higher range were mounted on the axles and those with lower range – on the tractor frame and the load deck of the trailer.

In each case the dynamic system was idealized as a system with one degree of freedom (see Figure 6b). Hence, stiffness k_i and damping coefficient c_i for each suspension system could be estimated based on free vibration theory as follows:

$$k_i = \frac{4\pi^2}{\tau_d^2} m_{bi} \tag{1}$$

$$c_i = 2 \frac{\delta}{\sqrt{4\pi^2 + \delta^2}} \sqrt{k_i m_{bi}}$$
(2)

$$\delta = \ln \frac{u_i}{u_{(i+1)}} \tag{3}$$

where: τ_d is the period of damped vibration; δ is the logarithmic damping decrement; m_{bi} is the tributary mass of the vehicle bodywork supported by the *i*-th axle; u_i and $u_{(i+1)}$ are two successive amplitudes.

The distance between the frame and the axle was measured using a linear displacement gage with the displacement changes registered every 0.005 second. Extracts from the displacement history with well-defined changes representing a pseudo-harmonic motion were selected to find the period and amplitude of damped vibration, as depicted in Figure 6c. Obtained values were averaged out and used for preliminary determination of the stiffness k_i and damping coefficient c_i .



Figure 6: Location of Sensors and Wooden Plank for the Front Suspension System (a) and its Idealized One Degree of Freedom Model (b) used for Preliminary Determining of the Stiffness and Damping Coefficient. Exemplary Results obtained from Experimental Test (c) – Distance Between the Frame and the Axle

The next step was to conduct dynamic tests for the actual vehicle which could provide data sufficient for validation of the complete FE model. During these tests the vehicle was driven over a speed bump with the speeds of 16, 24 and 32 km/h without load, and loaded with the speed of 8 and 16 km/h. Vertical accelerations a(t) at selected points and a change in distance between the axles and the frame u(t) were recorded as a function of time. Two standard speed bumps made of asphalt were used for the tests. Their shapes and dimensions allowed for obtaining the measurable range of vibration for representative points. The time histories of accelerations and distances obtained from the experimental tests were compared with the results from FE analyses. The spring and damping coefficients at all axles were adjusted as necessary until the performance of the FE model closely matched that of the actual vehicle.

FE ANALYSIS

The FE analyses were performed on the basis of nonlinear, explicit, dynamic LS-DYNA computer code. Only dynamic tests for the unloaded and loaded vehicle were simulated. The vehicle FE model was driven on the *Rigid Wall* part before it crossed the speed bump. It allowed reducing the CPU time of the each run because the computationally expensive contact between two deformable bodies was not included. Fully integrated (very fast) elements were used (LS-DYNA 2007). The time of the simulations was set to 5 seconds.

The motion of the FE model was executed in two phases. The *Initial Velocity Generation* keyword was used at the beginning of the analysis, whereas the *Boundary Prescribed Motion Set* keyword was applied to keep the constant velocity in appropriate range (LS-DYNA 2007). The *Database History* keyword was used to record the nodal point data for nodes corresponding to the selected points on the actual vehicle.

Selected results are presented in Figure 7 and Figure 8. Several analyses with the adjusted spring and damping coefficients obtained from the preliminary field tests were performed until the shape of both curves experimental and the FE analysis—were matched through a calibration process.

An effect of the speed bumps on dynamic behavior of a heavy vehicle was assessed numerically for three different speeds considered during the field tests: 16, 24 and 32 km/h without load. In addition, the speed of 48 km/h, not tested experimentally, was included in numerical analysis. A vertical force produced by the vehicle driven over the speed bump was calculated using FE analysis. Its value was related to the static load of the axle allowing determining the dynamic effect, as depicted in Figure 9. In addition, the spring forces were also extracted to estimate an influence of the speed bump on the suspension behavior. The result for the front suspension system is presented in Figure 9.



Figure 7: Comparison between Results of the FE Analysis with those obtained from Experimental Tests for the Front Suspension System: Change in Distance between Axle and Frame (a) and Vertical Acceleration of the Axle (b). Case No. 2: unloaded vehicle, speed of 24 km/h



Figure 8: Comparison between Results of the FE Analysis with those obtained from Experimental Tests for the Trailer Suspension System (Third Axle): Change in Distance between Axle and Frame (a) and Vertical Acceleration of the Axle (b). Case No. 2: unloaded vehicle, speed of 24 km/h



Figure 9: Ratio of the Dynamic to the Static Load of the Road caused by the Front Axle (a). The Spring Forces Variation of the Front Suspension System (b)

CONCLUSIONS

The best correlation can be observed for the front suspension system. This is due to the type of the suspension—leaf springs with the constant spring ratio—which was easy to simulate and to the relatively high axle load allowing a smooth and stable displacement history for the FE model validation.

Finding the correct values of spring and damping coefficients for the rear suspension system was the most difficult part. The difficulties were encountered especially during the preliminary tests and they were connected mainly to the sensitivity of the air springs and their susceptibility to the factors such as acceleration and breaking deceleration of the vehicle.

Based on the conducted tests the following conclusions can be formulated. The slow motion of the tested vehicle necessary for the preliminary tests should be executed by a different source, for example by another vehicle towing the tested one. That would allow avoiding uneven movements and jerks of the tested object. Moreover, the results would be more accurate if the tests were conducted on the vehicle with the engine turned off. The engine caused additional vibration which was detrimental to the final results.

Computer simulations can be efficiently used to assess dynamic reactions in pavements when vehicles are driven over the speed bumps. As institutively expected, these reactions are directly proportional to the vehicle speed. The same techniques can be used for other road and bridge surface imperfections and for qualitative assessment of dynamic impact factors for bridges.

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REAL TIME CONTROL FOR TIME DELAY SYSTEM

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KEYWORDS

delay system, PI controller, stability region, Hermit-Biehler theorem, optimization, genetic algorithm.

ABSTRACT

In this paper, we consider the control of time delay system by Proportional-Integral (PI) controller. By Using the Hermite-Biehler theorem, which is applicable to quasi-polynomials, we seek the stability region of the controller and the computation of its optimum parameters. We have used the genetic algorithms to lead the complexity of the optimization problem. An application of the suggested approach for real-time control on a heater PT - 326 was also considered.

INTRODUCTION

Systems with delays represent a class within infinite size largely used for the modelling and the analysis of transport and propagation phenomena (matter, energy or information)(Niculescu, 2001; Zhong, 2006). They naturally appear in the modelling of processes found in physics, mechanics, biology, physiology, economy, dynamics of the populations, chemistry, aeronautics and aerospace. In addition, even if the process itself does not contain delay, the sensors, the actuators and the computational time implied in the development of its control law can generate considerable delays (Niculescu, 2001). The latter have a considerable influence on the behaviour of closed-loop system and can generate oscillations and even instability (Dambrine, 1994).

PID controllers are of high interest thanks to their broad use in industrial circles (Cedric, 2002). Traditional methods of PID parameter tuning are usually used in the case of the systems without delays (Lequin et al, 2003; Liu et al, 2001). An analytical approach was developed in (Silva et al, 2005; Zhong, 2006) and allowed the characterization of the stability region of delayed systems controlled via PID. Indeed, by using the Hermit-Biehler theorem applicable to the quasipolynomials (Bhattacharyya, 1995; Silva et al, 2005), the authors have developed an analytical characterization of all values of the stabilization gains (K_p , K_i , K_d) of the regulator for the case of first order delay system. The same technique is used to provide a complete characterization of all P and PI controller that stabilize a first order delay system which considered as less complicated than the PID stabilization problem (Silva et al, 2000). In order to have good performances in closed loop, it is necessary to suitably choose the parameters of the regulator in the zone stability.

In this work, we look for optimum regulators under different criteria and we present the results of this approach when applied to the temperature control of a heater air stream PT - 326.

This paper is structured as follows: in section 2, we present the theorem of Hermit-Biehler applicable to the quasi-polynomials. Section 3 is devoted to the problem formulation for first order delay system controlled via PI controller. In order to obtain optimal regulator in the zone of stability, a description of the genetic algorithms is presented in section 4. Section 5 is reserved for real time example to test the control method.

PRELIMINARY RESULTS FOR ANALYZING TIME DELAY SYSTEM

Several problems in process control engineering are related to the presence of delays. These delays intervene in dynamic models whose characteristic equations are of the following form (Silva et al, 2002, 2005):

$$\delta(s) = d(s) + e^{-L_1 s} n_1(s) + e^{-L_2 s} n_2(s) + \dots + e^{-L_m s} n_m(s)$$
(1)

Where: d(s) and n(s) are polynomials with real coefficients and L_i represent time delays. These characteristic equations are recognized as quasi-polynomials. Under the following assumptions:

One can consider the quasi-polynomials $\delta^*(s)$ described by :

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$$\delta^{*}(s) = e^{sL_{m}}\delta(s)$$

= $e^{sL_{m}}d(s) + e^{s(L_{m}-L_{1})}n_{1}(s)$ (3)
+ $e^{s(L_{m}-L_{2})}n_{2}(s) + ... + n_{m}(s)$

The zeros of $\delta^{(s)}$ are identical to those of $\delta^{*}(s)$ since e^{sL_m} does not have any finite zeros in the complex plan. However, the quasi-polynomial $\delta^{*}(s)$ has a principal term since the coefficient of the term containing the highest powers of s and e^s is nonzero. If $\delta^{*}(s)$ does not have a principal term, then it has an infinity roots with positive real parts (Bhattacharyya, 1995; Silva et al, 2005).

The stability of the system with characteristic equation (1) is equivalent to the condition that all the zeros of $\delta^*(s)$ must be in the open left half of the complex plan. We said that $\delta^*(s)$ is Hurwitz or is stable. The following theorem gives a necessary and sufficient condition for the stability of $\delta^*(s)$ (Silva et al, 2000, 2001, 2002, 2005).

theorem 1 Let $\delta^*(s)$ be given by (3), and write:

$$\delta^*(j\omega) = \delta_r(\omega) + j\delta_i(\omega) \tag{4}$$

where $\delta_r(\omega)$ and $\delta_i(\omega)$ represent respectively the real and imaginary parts of $\delta^*(j\omega)$. Under conditions (A_1) and (A_2) , $\delta^*(s)$ is stable if and only if:

1: $\delta_r(\omega)$ and $\delta_i(\omega)$ have only simple, real roots and these interlace,

2: $\delta'_i(\omega_0)\delta_r(\omega_0) - \delta_i(\omega_0)\delta'_r(\omega_0) > 0$ for some w_0 in $[-\infty, +\infty]$

where $\delta'_r(\omega)$ and $\delta'_i(\omega)$ denote the first derivative with respect to w_0 of $\delta_r(\omega)$ and $\delta_i(\omega)$, respectively.

A crucial stage in the application of the precedent theorem is to verify that and have only real roots. Such a property can be checked while using the following theorem (Silva et al, 2000, 2001, 2002, 2005).

theorem 2 Let M and N designate the highest powers of s and e^s which appear in $\delta^*(s)$. Let η be an appropriate constant such that the coefficient of terms of highest degree in $\delta_r(\omega)$ and $\delta_i(\omega)$ do not vanish at $\omega = \eta$. Then a necessary and sufficient condition that $\delta_r(\omega)$ and $\delta_i(\omega)$ have only real roots is that in each of the intervals $-2l\pi + \eta < \omega < 2l\pi + \eta, \ l = l_0, l_0 + 1, l_0 + 2...$ $\delta_r(\omega)$ or $\delta_i(\omega)$ have exactly 4lN + M real roots for a sufficiently large l_0 .

PI CONTROL FOR FIRST ORDER DELAY SYS-TEM

We consider the functional diagram of figure 1, in which the transfer function of delayed system is given by (5)

$$G(s) = \frac{K}{1+Ts}e^{-Ls}$$
(5)

Where K, T and L represent respectively the state gain, the constant time and the time delay of the plant. These three parameters are supposed to be positive.



Figure 1: Closed-loop control of a time delay system

The PI Controller is described by the following transfer function:

$$C(s) = K_p + \frac{K_i}{s} \tag{6}$$

Our objective is to analytically determine the region in the (K_p, K_i) parameter space for which the closed-loop system is stable.

theorem 3

The range of K_p value, for which a solution to PI stabilization problem for a given stable open-loop plant exists, is given by (Silva et al, 2000, 2001, 2002, 2005):

$$-\frac{1}{K} < K_p < \frac{T}{KL} \sqrt{\alpha_1^2 + \frac{L^2}{T^2}}$$
 (7)

Where α_1 the solution of the equation $tan(\alpha) = -\frac{T}{L}\alpha$ in the interval $[\frac{\pi}{2}, \pi]$

Proof The closed loop characteristic equation of the system is given by:

$$\delta(s) = (KK_i + KK_p s)e^{-Ls} + (1+Ts)s \quad (8)$$

we deduce the quasi-polynomials:

$$\delta^*(s) = e^{Ls}\delta(s) = (KK_i + KK_p s) + (1+Ts)se^{Ls}$$
 (9)

substituting s=jw , we have: $\delta^*(j\omega)=\delta_r(\omega)+j\delta_i(\omega)$ where:

$$\begin{cases} \delta_r(\omega) = KK_i - \omega \sin(L\omega) - Tw^2 \cos(L\omega) \\ \delta_i(\omega) = w \left[KK_p + \cos(L\omega) - Tw \sin(L\omega) \right] \end{cases}$$
(10)

Clearly, the parameter K_i only affects the real part of $\delta^*(j\omega)$ whereas the parameter K_p affects the imaginary part. According to the first condition of theorem 1, we should check that the roots of δ_i and δ_r are simple. By using the theorem 2, while choosing, M = 2, N = l = 1 and $\eta = \frac{\pi}{4}$, we observe that $\delta_i(\omega)$ has simple roots for any K_p checking (7) (Bhattacharyya, 1995; Silva et al, 2005).

the application of the second condition of theorem 2, led us to:

$$\begin{split} E(\omega_0) &= \delta_i'(\omega_0)\delta_r(\omega_0) - \delta_i(\omega_0)\delta_r'(\omega_0) > 0\\ \text{for } \omega_0 &= 0 \text{ (a value that annul } \delta_i(\omega)) \text{ we obtain:}\\ E(\omega_0) &= (\frac{KK_p+1}{L})KK_i > 0 \text{ which implies } K_p > \frac{-a_0}{K}\\ \text{since } K > 0 \text{ and } K_i > 0. \end{split}$$

This proofs the first inequality given by(2)in Theorem 1. We consider that $z = L\omega$, we get:

$$\delta_r(z) = K \left[K_i - \frac{z}{KL} (\sin(z) + \frac{T}{L} z \cos(z)) \right] \quad (11)$$

It results that $a(z) = \frac{z}{KL}(\sin(z) + \frac{T}{L}z\cos(z))$ then

$$\delta_r(z) = K \left[K_i - a(z) \right] \tag{12}$$

for $z_0 = 0$, we obtain :

$$\delta_r(z_0) = K(K_i - a(0)) = KK_i > 0$$
 (13)

for $z_j \neq z_0, j = 1, 2, 3...$, we obtain:

$$\delta_r(z_j) = K(K_i - a(z_j)) \tag{14}$$

Interlacing the roots of $\delta_r(z)$ and $\delta_i(z)$ is equivalent to $\delta_r(z_0) > 0$ (since $K_i > 0$), $\delta_r(z_1) < 0$, $\delta_r(z_2) > 0$... We can use the interlacing property and the fact that $\delta_i(z)$ has only real roots to establish that $\delta_r(z)$ possess real roots too. From the previous equations we get the following inequalities:

$$\begin{cases}
\delta_r(z_0) > 0 \\
\delta_r(z_1) < 0 \\
\delta_r(z_2) > 0 \\
\delta_r(z_3) < 0 \\
\vdots \\
\vdots
\end{cases}$$

$$\begin{cases}
K_i > 0 \\
K_i < a_1 \\
K_i > a_2 \\
K_i < a_3 \\
K_i > a_4 \\
\vdots
\end{cases}$$
(15)

where the bounds a_j for j = 1, 2, 3... are expressed by:

$$a_j = a(z_j) \tag{16}$$

Now, according to these inequalities, it is clear that we need only odd bounds (which to say a_1,a_3). It has to be strictly positive to get a feasible range for the controller parameter K_i . From (Silva et al, 2000, 2002), a_j is positive (for the odd values of j) for every K_p verifying (7). Hence, the conditions giving by (15) are reduced to:

$$0 < K_i < \min_{j=1,3,5\dots} \{a_j\}$$
(17)

Once the stability domain is determined, the question is what are the optimum parameters of the PI controller which guarantee the good performance of the closedloop system? On the following, the genetic algorithm is proposed to answer this need.

GENETIC ALGORITHMS

The Genetic Algorithms (AGs) are iterative algorithms of global search of which the goal is to optimize a specific function called criterion of performance or cost function (Godelberg, 1991). In order to find the optimal solution of a problem by using AGs, we start by generating a population of individuals in a random way. The evolution from one generation to the following is based on the use of the three operators' selection, crossover and mutation

which are applied to all the elements of the population (Godelberg, 1991). Couples of parents are selected according to their functions costs. The crossover operator is applied with a P_c probability and generates couples of children. The mutation operator is applied to the children with a P_m probability and generates mutant individuals who will be inserted in the new population. The reaching of a maximum number of generations is the criterion of stop for our algorithm. Figure 2 shows the basic flow chart of AGs. The principle of regulator parameters opti-



Figure 2: Steps of the genetic algorithm evolution

mization by the genetic algorithms is shown by figure 3.



Figure 3: The optimization principle by genetic algorithm

In our case, we are interest to search the optimum controller parameters in the area of stability using one of following criterion *ISE*,*IAE*,*ITAE* and *ITSE* described by relation (23):

$$ISE = \sum_{0}^{t_{\text{max}}} e(t)^{2}$$

$$IAE = \sum_{0}^{t_{\text{max}}} |e(t)|$$

$$ITAE = \sum_{0}^{t_{\text{max}}} t |e(t)|$$

$$ITSE = \sum_{0}^{t_{\text{max}}} te(t)^{2}$$
(18)

If we want to minimize the tuning energy, the ITAE and the IAE criteria are considered. In the case where we privilege the rise time, we take the ITSE criterion. In order to guarantee the tuning energetic cost, we choose the ISE criterion (Villain, 1996).

The calculation steps of the control law are summarized by the following algorithm:

- 1. Introduction of the following parameters:
 - max_{pop}individuals number by population
 - initial population
 - *genmax* generation number
- 2. Initialization of the generation counter (gen = 1)
- 3. Initialization of the individual counter (j = 1)
- 4. For t = 1s to $t = t_{max}$ efficiency evaluation of j^{th} population individual $fitness(J) = \frac{1}{1+J}$
- 5. Individual counter incrementing (j = j + 1).
 - If $j < max_{pop}$, going back to step 4
 - If not: application of the genetic operators (selection, crossover, mutation) for the founding a new population
- 6. Generation counter incrementing (gen = gen + 1), If, going back to step 3.
- 7. taking $K_p opt$ and $K_i opt$ which correspond to the best individual in the last population (individual making the best fitness).

On the following, the genetic algorithm characterized by generation number equal to 100, $P_c = 0.8$, $P_m = 0.08$ and individual number by population equivalent to 20.

APPLICATIONS

This section presents an application example for the temperature control of an air stream heater (process trainer PT - 326), figure 4. This type of process is found in many industrial systems such as furnaces, air conditioning, etc. The PT - 326 has the basic characteristics of a large plant, with a tube through which atmospheric air is drawn by a centrifugal blower. Before being released into the atmosphere, air becomes heated by passing into a heater grid. Temperature control is realized by varying the electrical power supplied to the heater grid. Air is pushed through a tube by a fan blower and heated at the inlet. The mass flow of air through the duct can be adjusted by setting the opening of the throttle. There is an energized electric resistance inside the tube. Heat, due to the Joule effect, is released by resistance and transmitted by convection

This process can be characterized as a linear time delay system. Time delay depends on the position of the temperature sensor element that can be inserted into the air stream at any one of the three points throughout the



Figure 4: PT-326 heat process trainer

tube, spaced at 28, 140 and 280 mm from both the heater and the damper position. The system input, u(t), is the voltage applied to the power circuit feeding the heating resistance, and the output,y(t), is the outlet air temperature, expressed by a voltage, between -10 and 10V. the PT - 326 heating process is shown in figure 5.



Figure 5: Schematic illustration

The behavior of the PT - 326 thermal process is governed by the balance of heat energy. When the air temperature inside the tube is supposed to be uniform, a linear delay system model can be obtained. Thus, the transfer function between the heater input voltage and the sensor output voltage can be obtained as: $\frac{y(s)}{u(s)} = \frac{K}{1+Ts}e^{-Ls}$

For the experiment, the damper position is set to 30, and the temperature sensor is placed in the third position. The measurements acquisition is done by "PCI - DAS1002" card's, the sampling time is taken equal to $T_e = 0.03$ second. This choice takes account of the time computing and the constant time of the plant. Firstly data is taken by operating the heater open loop with square input 0V/2V as shown as figure 6. The data is then used to obtain models to represent the plant An enlargement of the first step response up to 1000 iterations is shown in the following figure. We define: Step1: step response up to 1500 iterations

Step3: step response from 3000 up to 4500 iterations Step5: step response from 6000 up to 7500 iterations Step7: step response from 9000 up to 1000 iterations

The transfer's functions corresponding to each step response are estimated by conventional graphical method;



Figure 6: Square input 0V/2V and outputs of PT - 326



Figure 7: First step response for PT - 326

and they are represented in table 1. So the PT - 326

Table 1: system parameter

	Step 1	Step 3	Step 5	Step 7	mean
L	0.57	0.6	0.54	0.54	0.5625
K	0.587	0.586	0.5872	0.5872	0.5869
T	1.572	1.5671	1.572	1.572	1.572

is described by the following transfer function: $\frac{y(s)}{u(s)} = \frac{0.58}{1+1.57s}e^{-0.56s}$

In order to determine K_p values, we look for α in interval $[0, \pi]$ satisfying $\tan(\alpha) = 2.89\alpha \Rightarrow \alpha = 1.764$. K_p range is given by: $-2 < K_p < 8.25$. The system stability region, obtained in plane is presented in figure 8. From figure 8, our K_p and K_i population's individuals are choosing between [-2, 8.25] and [0, 7.45]. PI controller optimum parameters supplied by genetic algorithm are presented by the following table. The following

Table 2: optimum PI parameters

criterion	ISE	IAE	ITAE	ITSE
$K_p opt$	3.67	3.33	2.94	3.95
$K_i opt$	4.24	4.36	4.04	4.33

algorithm describes the real-time implementation of the PI control law:



Figure 8: PI controller stability domain for PT - 326

- 1. Initialization, k = 1
- 2. Output acquisition y(k)
- 3. Error computation $e(k) = y_c(k) y(k)$
- 4. Control law Computation $u(k) = u(k-1) + K_p e(k) + (K_i T_e - K_p) e(k-1)$
- 5. Application of the control law u(k) to the process
- 6. Exhausting of the sampling time, k = k + 1 then go to step 2.

The followings figures show the responses of the closed loop systems in the case of PI controller designed by the genetic algorithms as described in table 2.



Figure 9: Evolution of the output and the control law (Case: PI - ISE)

It is clear from these figures that the closed loop system is stable and the output y(k) tracks the step input signal. From Table 3 we conclude that the minimal variance of control law was generate by the PI - ISE controller.

 Table 3: performance comparison

	ISE	IAE	ITAE	ITSE
var(u(k))	2.6708	2.779	2.8728	2.7234



Figure 10: Evolution of the output and the control law (Case: PI - IAE)



Figure 11: Evolution of the output and the control law (Case: PI - ITAE)



Figure 12: Evolution of the output and the control law (Case: PI - ITSE)

CONCLUSION

In this work, we use the Hermit-Biehler theorem to compute the region stability for first order delay system controlled by PI regulator. Lastly, we were interested in search of optimal PI for a given performance criteria (*ISE*, *IAE*, *ITAE*, *ITSE*), inside the stability region. In regard to the complexity of the optimization problem, we used the genetic algorithms. The validation of these results was tested in real time temperature control.

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PARAMETERIZATION OF LASER BURNED SAMPLES AND ITS USAGE IN DATA DESCRIPTION AND SIMULATION

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KEYWORDS

Parameterization, laser burning, model, simulation, approximation, surface.

ABSTRACT

This paper describes the reasons and methods for parameterization of samples burned by a laser beam. At the beginning, it gives information about data acquisition and description. In the main part, the paper summarizes the basic set of parameters which describe the shape of a pulse. From these parameters the basic shape is generated according to a mathematical description. The method of sample approximation is described in detail. Finally, the future plans are outlined.

INTRODUCTION

Our work is a part of a larger project that deals with laser burning, its control, and simulation of the process of laser burning. Simulation of the burning process should prevent real burning of pointless experiments. As an input into the simulation model real burned and measured data sets are used, but samples have to be processed first. We are interested in data preprocessing and its visualization. For our work, we use real samples burned into several materials and measured by a confocal microscope. The way of data acquisition is described in the following section.

All measured samples are represented in the form of a height map. Its format is described later in section Data Description. Our task is to visualize the samples and to design algorithms for automatic preprocessing and comparison of samples which will be later used for simulation purposes. Because the height map is not an optimal format for all these operations that we need to perform, we try to describe the sample in a different way. To recognize differences and similarities among similar samples, we had to explore the real samples carefully. The results of this process are described in the first part of the Results section. Our goal is to find a set of parameters that would define a mathematical function approximating the shape of the pulse optimally and to get a parametrical description of sample roughness in all its areas.

If we are able to describe the real sample by a set of parameters, we can use the parameterization as a part of

the sample generating process. First, we generate the basic shape of the pulse. To get more realistic results, the smooth surface generated by the function can be further modified by usage of random surface modification. For that we plan to use methods of waves modulation as well as methods of noise generation. Because the main idea of this paper is the exploration of real samples, their parameterization and the generation of the basic pulse shape, these methods are only outlined in the section Future Plans.

After a careful exploration of real samples, we can try to find the dependence of their parameters on the number of laser pulses burned during the real sample creation. Finally, we should be able to compute parameters for any arbitrary sample and to generate its surface in the process of simulation. In other words, we should be able to simulate the appearance of any sample based only on a limited set of samples. The surface of a 3D function can be used for the generation of any pulse described by the set of parameters as a method of the sample simulation.

Data Acquisition

To get data for the simulation input, real samples have to be burned by an existing laser equipment into a real material and then to be measured. The set of the samples is called an experiment. One experiment contains data for one particular laser device and one particular material. It means that for each combination of a laser device and a material which are used for simulation, a special experiment has to be performed. Each experiment consists of samples burned by the laser into a single point in the material. The number of pulses goes in sequence, e.g. from 1 to 100 (in Figure 1, each pulse from the sequence is burned on a separate row).

1x	• • • •
2x	
5x	
10x	
30x	••••
100x	••••

Figure 1: Experiment Layout

After reburning the same pulse several times with keeping the same conditions, the results differ a little, so each pulse count is repeated several times in order to get

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an average result. These samples are placed side by side in a single row (one row in Figure 1 corresponds to similar pulses). All data we use is burned by a laser device BLS-100 (Nd:YAG solid-material, lamp-pumped laser with wavelength of 1064nm) into steel and cermet (a composite material composed of ceramic and metallic materials). Parameters of burning are as follows: laser power 100W, current 28A, width of the ray 0.01mm, diaphragm 1.8.

After the samples are burned, they have to be measured. For this purpose, the confocal microscope Olympus LEXT OLS3100 is used. During the measurement, just a part of the material with burned pulses is focused, scale and zoom factors are chosen, the material sample is scanned and the measured data is saved. For the output from the confocal microscope, text file (CSV) is used. The zoom is chosen according to the experience with the particular material.

Data Description

The CSV file contains a matrix of real numbers which represents the sample surface. The values express heights of intersection points in the uniform rectangular grid. This grid represents a height map which describes the surface of the sample (see Figure 2).



Figure 2: Height Map of a Measured Sample

The majority of samples which we use has the same size as the sample in Figure 2. Most of the sample surface is filled by the area that was affected by the laser beam; the real dimension of the sample is $256 \times 192 \mu$ m. The grid of height map is really fine; most common grid step in used data is 0.25μ m. It means that the surface of such sample is described by 1024×768 values.

Let's explore the process of laser burning and material ablation in detail. During the burning process, the surface of the material is exposed to an intense pulsed laser beam that creates a rapid rise in local temperature. The surface is warming up and the material starts to ablate. The material, which is ablated, redeposites around the irradiated area and damages the surrounding material. Finally, at the exposure site, a pit with a transition ring around it is left behind (Dahotre et al. 2008). The cross-section of sample can be seen in Figure 3.



Figure 3: Cross-Section of a Sample and its Description

As can be seen in Figure 4, the real samples can be visualized in various ways. Different approaches enable various opportunities and we can see different properties there. The confocal microscope itself enables the 3D visualization (see Figure 2). In Figure 4, two different approaches of the sample visualization by our tool are shown. The grayscale image in Figure 4a is used for the sample exploration combined with the vertical and horizontal cross-sections of the sample surface. It gives a good imagination about distribution of heights and depths in the surface. Figure 4b shows the result of our 3D viewer. It enables to explore the surface from an arbitrary position of the camera. Thanks to the plasticity and shades, the output is more realistic than the previous approach. The top view of the sample is shown in Figure 4b. In both these images, the same sample (100 laser pulses burned into a steel surface) is shown.



Figure 4: Visualization of a Sample: a) as a Grayscale Image, b) as a 3D View

Let's describe the sample surface in detail. The surface of the original material is quite smooth with some local roughness (Figure 5a), the centre of the pulse (i.e. the area irradiated by the laser beam) is also smooth and the bottom of the pit is a little bit rougher (Figure 5b). The most ragged surface part is the transition region. The surface is modulated by some concentric waves that are both regular and irregular (Figure 5c). Sometimes, local defects with a considerable roughness can appear, especially at the outer border of the transition ring (Figure 5d). They are caused by the ablated material that becomes cool and deposits in the area next to the pit irregularly. At the outer border, the roughness declines slowly and it goes into the roughness of the bulk material.

All these facts should be taken into account if we want to generate the surface of a pulse from its parameters. Samples burned into the same material are similar and some characteristics of the burned sample depend directly on the used material itself. If we burn the same sample twice, it will be never the same because at least the surface of the basic material differs. That is why it is not necessary to save the exact height map, but it is sufficient to save characteristics and attributes of the sample. It is the main reason for the parameterization of samples.



Figure 5: Typical Examples from Different Parts of a Typical Sample Surface

The set of sample parameters is described in the following section. If we want to generate the sample surface from these parameters, we have to, at the beginning, get the basic shape of the heat affected area. This procedure is described as the main idea of this paper in the section Pulse Surface Generating.

PULSE PARAMETERIZATION

To get information about the pulse shape, we use crosssection lines. Figure 6 shows the cross-section curves of four similar samples of steel with 100 pulses burned into one place. Because pulses are not symmetric, we cannot use cross-sections measured only in one direction. Our experiments show that cross-sections measured in two directions – in the broadest and the narrowest width of the pulse, are sufficient. Thanks to the character of pulses the cross-sections are often orthogonal and correspond to cross-section parallel to xand y axis. For simplification let's call them CS_X and CS_Y.



Figure 6: Vertical Cross-Section Lines of Four Similar Samples – 100 Laser Pulses Burned into the Steel

It is evident that all samples are most similar in the area of the pit. In Figure 6b, the shape of the pit is damaged by a local defect of the material, but still the correct shape can be guessed well. The surface of the pulse in the pit is quite smooth and the slight roughness is perceptible in the bottom part. On the contrary, the border of the pulse – the transition ring, which is formed by the melted material, is different for each explored case.

The aim of parameterization is to get a set of parameters that describes the sample sufficiently. Some of them depend on the material and so they do not have to be gained automatically (such parameters are marked with an asterisk in Table I), the others differ for each sample. The parameters can be grouped according to the area. The names of parameters used in the following description are given in parenthesis behind the description.

Table I: Parameters for the Sample Representation

basic	basic material level (materialLevel)
material	diameter, height and density of bumps *
pit	diameter (semimajor and semiminor axis of the ellipse) (a, b)
	ablation depth (pitDepth)
	roughness of the pit bottom *
transition	the half of the ring width (ringRadius)
ring	average height (ringHeight)
	waves description - count, diameter,
	height, width (will be not solved in this
	paper yet)
	parameters for local defects *

In the simplified cross-section line of the sample we can detect several important points. Points $A[x_A, y_A]$ and $B[x_B, y_B]$ state the outer border of the pulse pit, $A'[x_A, y_A]$ and $B'[x_B, y_B]$ determine the outer border of the transition ring. Point $S[x_S, y_S]$ gives position of the bottom of the pit. All points are shown in Figure 7. The symbols will also be used in the following computations.



Figure 7: Important Points in the Cross-Section Line

For the detection of these points algorithms for the pulse automatic detection described in (Hájková 2008) are also used. If the area of the pulse is detected, the crosssection lines from the broadest part of the pulse in both the vertical and the horizontal directions are used. From them, the points are derived. The level of basic material can be determined according to methods described in (Hájková 2008). The inner diameter of the ring corresponds to the diameter of the pit and the width of the transition ring is computed from the cross-section lines as in the case of the pit. The half of the ring width is called the ring diameter.

More problematic task is to compute the maximal height of the ring, because the surface of real samples is in this area very rough, so we cannot use only the maximal value of the ring cross-section. But if we discretize the quadratic function, we can compute the average value of the parabola. As can be seen in Figure 8, where the average value is shown as the dashed line, the result depends on the sampling frequency.



Figure 8: The Position of the Average Value in the Parabola Represented by a) 5 values; b) 21 values.

Because we need to compute the average height of the transition ring, we have to use the same frequency that was used previously for the cross-section of the pit. First, we compute the rate of the average value and the difference of the maximal and the minimal value (amplitude) in the discretized parabola and we get the relative position of the average value from the top of the parabola. This value is independent from the height multiplicator *a* of the parabola in the parabola definition $(f(x) = -ax^2)$. That is why we can use the expression (1) to compute the amplitude (the height) of the transition ring of the pulse.

$$\frac{functionAverage}{functionAmplitude} = \frac{ringAverage}{ringHeight}$$
(1)

PULSE SURFACE GENERATING

Because both parts of the pulse (i.e. the pit and the ring) differ quite a lot, we have decided to approximate them separately by two different functions and most especially to differentiate the way of surface roughness description. Both generated surfaces are finally connected into the final shape. In following sections the method is derived (Rektorys 1981), (Weisstein 1999).

Pit Approximation

After several experiments, it appears that the basic shape of the pit cross-section corresponds to the shape of the plot of a quadratic function. The cross-section can be interlaid by a parabola having the equation showed in the expression (2). The results of this parabolic approximation of the pulse pit can be seen in Figure 9.

$$y = \frac{y_A - y_S}{(x_A - x_S)^2} (x - x_S)^2 + y_S$$
(2)



Figure 9: Vertical Cross-Section Lines of Samples from Figure 6 and their Approximation by a Parabola

From the given points measured in both CS_X and CS_Y , we can compute the other characteristics of the pit, such as its depth (*pitDepth*) or diameters of the pit in the broadest (*a*) and the narrowest (*b*) place. As can be seen in Figure 10, in the real samples of 10, 50 and 100 laser pulses burned into steel, the pit has a circular or elliptical shape from the top view.



Figure 10: Samples of 10, 50 and 100 Laser Pulses Burned into the Steel from the Top View

If the pulse pit can be approximated by the parabola in its cross-section, the whole pit can be approximated by an elliptical paraboloid. Because we need the paraboloid going through the top border of the pit, the equation representing it has to be modified as in (3). The origin of the solid lies in $S[x_0, y_0, z_0]$, *pitDepth* represents the depth of the paraboloid and *a*, *b* are axis of the ellipse. The elliptical paraboloid is depicted in Figure 11.

$$z = pitDepth * \left(\frac{(x - x_0)^2}{a^2} + \frac{(y - y_0)^2}{b^2}\right) + z_0$$
(3)

Ring Approximation

The approximation of the area of pulse transition ring is much more problematic, because its shape is irregular and rough (as can be seen from samples in Figure 6). The material surface is created during the burning process by the ablated material that forms a ring on the border of the burned pit as the material is getting colder. To find the approximating function, we had to simplify it and then to find a suitable way of random noise generation to get as realistic results as possible.



Figure 11: Elliptical Paraboloid and its Parameters.

First, we had to find a suitable function that could be used for the approximation of the basic shape of the ring cross-section. We have decided once again to use the quadratic function. To find an appripriate parabola, we need several parameters to describe the ring. These are shown in Figure 12 – the ring radius and its maximal height and also the level of the basic material. If we have computed all these parameters, we can define the parabola according to the expression (4).



Figure 12: Important Parameters for the Description of the Ring Cross-Section

$$y = \frac{ringHeight}{ringRadius^{2}} * (x - a_{R})^{2} + ringHeight + materialLevel$$
(4)

The whole ring should be approximated by a 3D function. It seems to be roughly similar to the top half of a torus. A torus is a surface of revolution generated by revolving a circle in three dimensional space about an axis coplanar with the circle, which does not touch the circle. A torus is shown in Figure 13. Of course, for our purposes, it has to be modified.



Figure 13: A Torus.

Because the ring has an elliptical shape from the top view and the shape of a parabola from the cross-section, the solid representing the ring should be created as a surface of revolution generated by revolving a parabola along the elliptic trajectory in three dimensional space. The approximation of the whole ring can be done by the half of the parabolic elliptic torus. The ellipse and its axes are shown in Figure 14.



Figure 14: Description of the Ellipse Axis

Now we have to describe it mathematically. The ellipse is defined as (5), where u and v are the axis of the ellipse.

$$1 = \frac{(x - x_0)^2}{u^2} + \frac{(y - y_0)^2}{v^2}$$
(5)

The maximum of the parabola representing the ring has to be placed on this ellipse. We can define $u^2 = a_R$ and $v^2 = b_R$. For our case, we can use the equation (6).

$$p = \frac{(x - x_0)^2}{a_R} + \frac{(y - y_0)^2}{b_R}$$
(6)

The value p = 0 represents the center of the ellipse, p = 1 defines the ellipse itself. If p varies from 0 to 1, it represents the area bordered by the ellipse and all values p > 1 points outside the ellipse.

Next, we need an expression for distance of a point from another point. Morespecifically, we need to compute the distance of the processed point from the center $[x_0, y_0]$ during the surface generation. This distance has to be adjusted according to the ellipse and so for the next computed according to the expression (7) determines the distance of the parabola maximum from the center of the ellipse in a given direction (as can be seen in Figure 15).

$$d_T = \frac{\sqrt{(x - x_0)^2 + (y - y_0)^2}}{p}$$
(7)



Figure 15: Description of Distances: a) from the Top View, b) from the View of Ring Cross-Section

To get the right shape of the parabola, we have to compute the parameter k that will determine the opening of the parabola (8). It depends on the maximal ring

height and its radius that has to be recalculated by d_T to get the ratio to the ellipse distance.

$$k = \frac{ringHeight}{\left(\frac{ringRadius}{d_T}\right)^2}$$
(8)

Now we can substitute into the expression (4). Because we compute in recounted distance (in the interval <0, 1>) instead of the value a_R , we have to use the value 1. Finally, the torus is defined as (9). The constants ringHeight and materialLevel are added because of shifting the generated surface into the right height. Otherwise, it would be placed under the zero level.

$$z = -k * (p-1)^{2} + ringHeight + materialLe vel$$
(9)

RESULTS

In the first section of the results section, the parameter comparison of the real samples is made. In the second section, the results of the pulse approximation are shown, both in the form of pulse cross-section (Figure 17) and as the 3D view (Figure 18).

Pulse Parameterization

As a part of the parameterization process, we have to explore the real samples carefully. As written in the section Data Acquisition, the same number of laser pulses burned into the same material several times under the same conditions does not give the same results and that is why each pulse count burning is repeated several times. First, we need to know how much the similar samples differ. To show concrete numbers, the basic parameters computed for five similar samples with 100 laser pulses burned into the steel were summarized in Table II. Moreover, the average values for each single parameter are also computed.

Table II: Basic Parameters of Five Similar Samples [µm]

	а	b	pit depth	ring width	ring height
Α	39.0	43.13	8.44	13.66	2.68
В	38.37	44.25	9.89	14.5	1.99
С	39.63	44.38	8.94	12.63	1.93
D	38.13	46.38	8.5	12.35	1.51
Ε	43.88	46.0	9.39	12.63	3.89
average	39.8	44.83	9.0	13.15	2.4

Although the similar samples differ, the parameters describing the basic shape of the heat affected area do not differ a lot. That is why we can use the average values for generating the basic shape of the pulse pit and the transition ring. Our second aim is to get the information if there is any dependence between the number of the laser pulses burned into the material and the shape of the sample. We can have a look at the real values again. The computed parameters for the set of samples with 10, 30, 50, 70 and 90 laser pulses burned into steel are shown in Table III. The dependencies of the parameters on the number of burned laser pulses are plotted in Figure 16.

Table III: Basic Parameters of the Set of Samples [µm]

	а	b	pit depth	ring radius	ring height
10	21.0	25.13	3.81	16.41	2.8
30	23.75	24.0	3.45	19.25	2.42
50	32.38	35.88	6.47	13.78	2.3
70	37.25	42.0	9.27	11.38	3.21
90	40.25	46.13	7.08	10.91	2.3



Figure 16: Parameters Dependence Plot

Pulse Approximation

The approximation was tested on various samples. The results for the area of the pit are very successful. More problematic is the area of the ring, where the roughness of the sample surface is high.

Results of approximation of the sample with 100 laser pulses burned into steel can be seen in Figure 17. In Figure 17a-c), cross-sections in the horizontal direction are shown, in Figure 17d-f), vertical cross-sections can be seen. The first cross-section from each triplet represents the middle of the pulse in the given direction, the others move more to the margin.



Figure 17: Approximation of 100 Laser Pulses Burned into Steel - Cross-Section Lines

To compare the results in 3D view, see Figure 18. In the left column, the original samples are placed, the surface generated according to the parametric description is shown in the right column. For the comparison, samples with 10, 50, and 100 pulses burned into steel were chosen. All samples are watched from the same distance and direction.



Figure 18: 3D Views at the Original and Generated Samples of 10, 50 and 100 Pulses Burned into Steel

FUTURE PLANS, CONCLUSION

The method described in this paper can be used for approximation of samples by a simplified, mathematically described smooth surface. To get more realistic results, we have to enhance the sample generation with random features such as methods for generating noise or various defects.

We are already experimenting with some of them. Present experiments show that the use of Perlin noise generating function (Perlin 1985), (Perlin 2002) can be the solution. The current results can be seen in Figure 19. In Figure 19a-b, a part of the transition ring of two different samples with the local roughness is shown, in Figure 19c, the surface generated by the Perlin noise function is depicted.

We are also testing number of further methods, e.g. modulation of concentric waves (irregular waves in a real sample can be seen in Figure 5c.), distortion, etc.

Of course for all these methods we need various parameters which would define roughness of the surface or the frequency of the local defects. Our task is also to design methods for an automatic parameterization of samples.



Figure 19: a-b) Local Defects of Two Different Samples, c) Surface Generated by the Perlin Noise Function

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MULTI-DOMAIN MODELLING - AN ADVANTAGE IN MODELLING, SIMULATION AND CONTROL EDUCATION

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KEYWORDS

Multi-domain modelling, object oriented modelling, helicopter, control systems

ABSTRACT

The paper deals with an important aspect of continuous systems modelling and simulation approaches, with possibilities for multi-domain modelling. The traditional approach is based on block oriented schemes in which causal relations play an important role. However this causality is artificially generated in order to fulfil appropriate conditions for simulation on conventional sequential computers. Fortunately new concepts which are based on object oriented approaches, physically oriented connections and algebraic manipulations enable the so called acausal modelling which can efficiently be used for multi-domain modelling. The advantages and disadvantages of traditional and more advanced approaches are discussed.

The described multi-domain approach is illustrated with modelling of a laboratory helicopter using a very popular multi-domain modelling environment Dymola with Modelica language. A multivariable controller was designed for a wide operating range. The control signals which drive the main and the tail rotors enable the desired pitch and rotation (azimuth) angles. The multidomain object oriented approach enables an efficient coupling of elements from mechanical libraries and a block library for the implementation of control system.

INTRODUCTION

Standardization of languages for modelling and simulation was always very important in the history. However the last standard that was really accepted was CSSL standard (Strauss 1967). Nowadays perhaps the most promising activities are in conjunction with the so called Modelica activities (*www.modelica.org*). After an initiative of the Federation of European Simulation Societies EUROSIM and The Society for Computer Simulation SCS in the middle of nineties a new language Modelica (Modelica 2005, Fritzson 2004), which gives

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) a hope to become a kind of international standard for model exchange, was defined.

A lack of object-oriented properties, which disables the reuse of already build models, is an important disadvantage of many modern modelling and simulation tools. Due to this reason some special-purpose tools were developed (for mechanical, electrical, chemical systems,...). In modelling of complex industrial systems however combinations of systems from different areas, i.e. multi-domain systems, are frequently needed (e.g. mechanical, electrical, hydraulic as well as control systems in mechatronics, particularly within automotive, aerospace and robotics applications). There were many attempts to connect different modelling tools, however the more efficient approach is to use tools which support multi-domain modelling (Van Beck and Roda 2000). Modelica with appropriate working environment e.g. Dymola (Cellier 1991, Dymola 2008) is probably the most promising multi-domain modelling environment based on object oriented approach and 'physical' way of connections between model components.

IMPORTANT FEATURES OF ADVANCED OO ENVIRONMENTS

Block oriented approach versus object oriented modelling and simulation approach

In order to allow the reuse of component models, the equations should be stated in a neutral form without consideration of computational order. This is so called acausal modelling (Zupančič et al. 2005, Zupančič and Sodja 2008). However most of the general-purpose simulation software on the market such as ACSL, Simulink,... assume that a system can be decomposed into block diagram structures with causal interactions (Matko et al. 1992, Cellier 1991). In this procedure state derivatives must be expressed which leads to the explicit state space form

$$\dot{x} = f(x, u, t) \tag{1}$$
$$y = g(x, u, t)$$

which can be efficiently simulated with ODE solvers. u is an input, y is an output and x is a state. It is rare that a natural decomposition into subsystems leads to such a model. Often a significant effort in terms of analysis and analytical transformations is needed to obtain a problem in this form. It requires a lot of engineering skills and manpower and it is error-prone.

In Modelica and some other multi-domain modelling tools it is possible to write balance and other equations in their natural form as a system of differential-algebraic equations, DAE

$$0 = f(\dot{x}, x, y, u, t) \tag{2}$$

where x is the vector of unknowns that appears differentiated in the equation and y is the vector of unknowns that do not appear differentiated. Computer algebra is utilized to achieve as efficient simulation code as possible, similar when we convert the equations 'manually' into ODE form.

Object orientation

We shall not talk about general concepts in OO programming where well known terms as encapsulation, data abstraction, inheritance, dynamic binding, ... are used. From a modeller point of view, OO means that one can build a model similar to real system: taking a pump, a pipe, a valve, ... and connecting them. For an efficient modelling, modelled systems are decomposed into subsystems (components), which are modelled as submodels and then hierarchically connected into a complete model. Modelling languages enable simple reuse of already build models. To reuse a certain model in other models it should be defined as a class. Model classes can be defined by physical laws (energy and mass balance equations and not necessarily with state space description (Equation 1). This contributes to a better understanding and reusability of models.

'Physically' oriented connections

The appropriate complexity of the implementation of the connections between model components (classes) is probably the most important property of multi-domain OO modelling tools. Connections between submodels are based on variables, which define proper relations and influences between movements, angles, currents, pressures, torques, forces, etc. It is similar as when real systems are built. Figure 1 shows how three mechanical rotational subsystems M1, M2 and M3 are connected. Several physical variables are presented in connections (connectors in Modelica):

- τ_i torques
- θ_i angles

- ω_i angular velocities
- α_i angular accelerations



Figure 1: Connection of three mechanical subsystems

In general there are two types of variables, which are defined in connectors of subsystems: variables that become equal in connection points, in our example angles, velocities, accelerations (ACROSS variables, also potential, temperature, pressure in other types of systems)

$$\theta_{I} = \theta_{2} = \theta_{3} \qquad \omega_{I} = \omega_{2} = \omega_{3} \qquad \alpha_{I} = \alpha_{2} = \alpha_{3}$$
(3)

and variables which sum equals zero (THROUGH variables, in our example this is torque, but also current, force etc. in other systems - prefix FLOW in Modelica)

$$\tau_1 + \tau_2 + \tau_3 = 0 \tag{4}$$

CONNECTOR is a special structure in which all the variables are collected. Each CONNECTOR has a name, which is composed of a submodel name and a name of a particular connector. Connections in traditional block diagram simulation languages can be treated as a subset of connections introduced by connectors. Namely they possess only variables of the type ACROSS, which become equal in junction points.

Example of a connector definition in Modelica

connector flange
 Real theta,omega,alfa; // Type across
 flow Real tau; // Type through
end flange;

By joining connectors the submodels are connected. During processing the modelling tool automatically generates equations 3 and 4 from submodel connector definitions.

Summary of features of Multi-domain OO modelling and simulation environments

Some important features of modern multi-domain OO modelling and simulation environments (e.g. Dymola with Modelica) are:

• Modelling of various kinds of complex physical systems with object oriented approach.

- Multi-domain tools, equivalently usable for modelling of mechanical, electrical, chemical, thermo dynamical and other systems.
- Possibilities to reuse already built models.
- Acausal model building.
- Hierarchical structure of models.
- Description of processes through physical laws (differential equations) irrespective to the type and purpose of a model.
- Easy and efficient way for submodels connections through connectors (more general then input-output connections known in block oriented simulation tools).
- Symbolical and numerical solving of systems of equations algebraic formula manipulation.

Modelica - OO modelling standard

Modelica (Modelica 2005, Fritzson 2004) is a modelling language which supports both high level modelling using pre-prepared complex model components and detailed modelling by equations. Graphical diagram layer and textual layer can be efficiently combined. The basic construct in Modelica is class. There are several types of classes with several restrictions: class, model, block, function, package, type etc. There are already several pre-prepared packages or libraries in standard Modelica library, e.g. for block diagrams, for electrical and electronic systems, for mechanical systems, for thermal and some others. Many other libraries are public domain libraries. In the past we developed a Modelica process systems library (Zupančič et al. 2005). However in this paper we focus to the mechanical systems which are even more appropriate for theoretical modelling as process systems (systems with level, flow, pressure, temperature, flow, PH, ..) and therefore very convenient to show the advantages of multi-domain object oriented acausal modelling.

EXAMPLE: MODELLING OF A LABORATORY HELICOPTER

The advantage of the multi-domain OO modelling will be shown with a modelling and control of a laboratory helicopter device. Laboratory set-ups, which model real processes, and mathematical models have a significant role in efficient control design and education. The CE150 (Figure 2) is a laboratory helicopter made by Humusoft (Humosoft 2002). It is used for studying system dynamics and control engineering principles and enables a wide range of practical experiments. The goal of modelling and identification is to prepare a basis for the students' laboratory assignments, such as designing a multivariable controller that ensures satisfactory control in the wide operating range. There are two well known modelling approaches: theoretical and experimental. In helicopter modelling both approaches were combined. The mathematical model is described in details in Karer and Zupančič 2006.

The laboratory helicopter set-up comprises a helicopter body carrying two motors, which drive the main and the tail rotors and a servomechanism, which shifts the centre of gravity by moving a weight along the helicopter's horizontal axis. The helicopter body is mounted to the stand so that two degrees of freedom are enabled:

- the rotation around the horizontal axis (pitch angle y_{ψ}) and
- the rotation around the vertical axis (rotation angle or azimuth y_{φ}).

Figure 2 depicts the helicopter as it finally appears in animation scheme in Dymola/Modelca environment. The model can be described as a nonlinear multivariable system with three inputs: the voltage driving the main rotor motor (u_i) , the voltage driving the tail rotor motor (u_2) and the voltage which drives the servomotor for positioning of the weight. In our case only the first two inputs are taken into control. The weight is positioned to a fixed place, defining the appropriate mechanical characteristic of the helicopter. The system has two outputs: pitch angle (y_{ψ}) and rotation angle (y_{φ}) . Forces which effect the helicopter body F_{main} , F_{react} and F_{tail} will be explained later.



Figure 2: Laboratory helicopter with forces affecting the body and control input/output signals

Multi-domain approach is useful because we combine two different areas: mechanical systems and control systems which are usually modelled with block diagrams. We chose *Modelica* (Modelica 2005, Fritzson 2004) as mechanical systems and block diagrams are included in the Standard Modelica library. *Dymola* environment (Dymola 2008) which supports *Modelica* was used. For animation the body of the helicopter and both rotors were drawn with program *SolidEdge* and with *DxfExport* add-in exported into *dxf* file format. *Dymola* uses *dxf* files to create an animation of model components. The helicopter body and the stand were modelled with the standard *Modelica* libraries *Mechanics\MultyBody and Mechanics\Rotational*.

The designed mechanical model was then used in Matlab/Simulink environment as Dymola block. Namely

Matlab/Simulink environment is very efficient for control system design as Control, Optimization or some other tools (toolbox) can be used. The control scheme designed in Matlab/Simulink was then implemented also in the *Dymola/Modelica* environment using standard *Modelica* libraries *Block\Continuous*, *Block\Sources* and *Block\Math*.

The overall scheme of the top level model in Dymola/Modelica is shown in Figure 3. The scheme is very clear. It consists of the coordinate system definition, the stand model, the helicopter body, the tail and main rotor model (rotor means motor and propeller) and the controller with two reference signals for pitch and rotation angle.



Figure 3: The top level model of the control system

Coordinate system

Coordinate system orientation is such that the gravitational force is in the direction of negative y axis. It is defined by the *Modelica* class *world*.

Model of the stand

The stand (see Figure 4) is modelled with translations (pure transformations of coordinates, straight lines between *a* and *b* connectors) and two bearings (actuated revolute joints *Revol_ext* and *Revol_ext1* in *Modelica*). Rotational axis of the first bearing is y axis (rotation in the horizontal plane) and of the second bearing is z axis (rotation in the vertical plane). The used actuated revolute joints were actually extended with additional outputs in order to get more simple and useful information about the pitch and rotation angles. Namely the connectors of revolute joint have a complex information about movements and velocities with three components in (*x*,*y*,*z*) coordinate system. In this way the angle sensors of the set-up were modelled. The bearing

friction was modelled using *bearingFriction* blocks, where characteristics of the friction are described with lookup tables. The functions for both friction characteristics were defined using relation

$$\tau_{friction} = B_1 \omega + B_2 sign(\omega) \tag{5}$$

in which linear and Coulomb part are taken into account. The relation (5) was implemented with lookup tables in both bearing friction classes.



Figure 4: The stand model

The coordinate system is connected to the connector *world* and the body of the helicopter is connected to the connector *helicopter body*. Translations fT2 and fT3 do not influence the dynamics. They are inserted for more realistic animation for the rotational axis in z direction.

Model of the helicopter body

The central part of this model class (see Figure 5) is the model class BodyShape from the MultyBody library which is suitable for rigid body modelling. We have to specify the vector from frame *a* to frame *b* resolved in frame a, the vector from frame a to the centre of mass, resolved in frame *a* and the mass of the rigid body. Beside we have to specify also the inertia tensor with J_{xx} , J_{yy} , J_{zz} , J_{yx} , J_{zx} , J_{zy} . The inertia tensor has to be defined with respect to a coordinate system that is in the origin of the centre of mass of the body. In our example we had to identify and took into account J_{yy} and J_{zz} . With the series of translations (fTy, fTrx, fTry, fTrz) we adequately moved the rotors from the rigid body connectors so that the generated forces produced by rotors had the right levers. In BodyShape model class the animation shape can be selected. In our case the shape was drawn with a program SolidEdge. The drawing was exported to the dxf file format. This file was then chosen in the animation options of the BodyShape class. Unfortunately Dymola cannot interpret the dimensions of objects in dxf files. Therefore we added to the model a set of translations for the proper animation (the encircled part in Figure 5).



Figure 5: The helicopter body model

Determination of parameters

Modelling in Dymola/Modelica environment is actually a kind of theoretical modelling with a strong support of Modelica libraries. However many parameters have to be experimentally determined. Some experiments were very simple geometrical measurements, some others were more sophisticated. The approaches and the parameter values are presented in more details in Karer and Zupančič 2006. In this paper we shall briefly described only some more sophisticated procedures.

The centre of gravity was determined with some simple mechanical experiments for a predetermined position of the weight which enable the changeable dynamic properties.

For both bearings the constants B_1 and B_2 , the moment of inertia tensor J of the regid body were derived with the minimization of criterion function (6), which takes into account the integral of the square difference between the real response y_{real} and the model response y_{mod} with different experiments with appropriate input signals u_1 and u_2 and appropriate initial conditions.

$$\min_{J,B_1,B_2} \int_{0}^{t_{\max}} (y_{real}(t,u_1,u_2) - y_{mod}(t,u_1,u_2))^2 dt \quad (6)$$

Nelder-Mead optimization method in Matlab was used.

Dynamics in one rotational direction (in one plane) was determined when the movements in another plane was disabled. For rotation around around horizontal axis (movements in vertical plane) we obtain

 $J_{zz} = 2.43 \cdot 10^{-3} kg m^2$ $B_{1z} = 1.53 \cdot 10^{-4} kg m^2 s^{-1}$ $B_{2z} = 1.03 \cdot 10^{-4} kg m^2 s^{-1}$

and for rotations around vertical axis (movements in horizontal plane)

 $J_{yy}=2.02 \cdot 10^{-3} \ kg \ m^2$ $B_{1y}=5.52 \cdot 10^{-4} \ kg \ m^2 s^{-1}$ $B_{2y}=5.96 \cdot 10^{-4} \ kg \ m^2 s^{-1}$

Model of rotors

Each rotor generates two forces that affect the movements of the helicopter body (see Figure 2). The first force is the 'useful' propulsation force in the direction of rotational axis (F_{main} of the main rotor and F_{tail} of the tail rotor). The second force is a reaction force, which is perpendicular to the rotational axis and acts as a kind of disturbance being a consequence of the rotor rotations and air resistance (F_{react} of the main rotor, the reaction force of the tail rotor is neglected). The reaction force of the main rotor must be compensated by the propulsation force of the tail rotor. There is also a gyroscopic effect caused by rotation of the main rotor which effects the additional torque around the horizontal axis which was neglected in our study. From this short discussion we conclude that we need a multivariable control approach as each control input influences both outputs (especially u_l).

The propulsation forces can be modelled mathematically using appropriate equations for interactions among the air, the shape and rotational speed of the rotor or as in our case they can be modelled experimentally. To model the forces we used experimentally obtained transfer function (7) of second order with double pole and the output quadratic nonlinearity (10)

$$\frac{U_m(s)}{U(s)} = \frac{1}{(Ts+1)^2}$$
(7)

$$F_{prop} = au_m^2 + bu_m \tag{8}$$

In Equation (7) U is the voltage driving the rotor motor $(U_1 \text{ or } U_2)$ and F_{prop} in Equation (10) is the useful force of the rotor $(F_{main} \text{ or } F_{tail})$. Parameters a and b are gained from the static characteristic.

We modelled the reaction force similar to the propulsion force except that we introduced more complex numerator dynamics (11)

$$\frac{U_m(s)}{U(s)} = \frac{T_{1r}s^2 + T_{2r}s + 1}{(Ts+1)^2}$$
(9)

$$F_{react} = a_r u_m^2 + b_r u_m \tag{10}$$

For the main rotor the parameters are: a=2.488 N, b=0.992 N, T=0.094 s, $T_{1r}=0.0017 s$, $T_{2r}=0.1908 s$, $a_r=0.296 N$, $b_r=0.2 N$ and for tail rotor: a=0.792 N, b=0.316 N, T=0.094s.

The block diagram, which realizes the forces for the main rotor (Eqs. 7-10) is shown in Figure 6.

Figure 7 describes the model of the rotor. The part that is outside the encircled area is actually the part described in Figure 6 which calculates the forces. The encircled part is for the animation purposes. For this purpose we model a bearing and a rotor with no mass. These parts do not affect the model dynamics. The rotational speed of the rotor is proportional to the voltage on the motor.







Figure 7: The model of rotors

Controller

The control system was designed using Matlab/Simulink environment. In Simulink the overall mechanical model was presented with the so called Dymola block. The simulation scheme is depicted in Figure 8. The input u_1 into the helicopter model is the voltage driving the front rotor and the input u_2 is the voltage driving the tail rotor. These are control signals. Output y_1 is the pitch angle and y_2 is the rotation angle. These are controlled signals.

Both control loops are combinations of the feedforward control and the PID feedback control with windup protection. Feedforward signals are obtained from the reference signals *Ref1* and *Ref2* which are processed with two nonlinear functions which are realized with two lookup tables. The feedforward signals bring the controlled signals into the vicinity of the reference signals. Fine corrections and steady state error eliminations are achieved with appropriately tuned PID controllers.

As the emphasize of this paper is given to the multidomain object oriented modelling approach we shall not describe the controller tuning procedure and the appropriate parameters of the control system.



Figure 8: The control system in Matlab/Simulink environment

Figure 9 shows the time responses of the pitch and rotation signals. The reference of the pitch angle was chosen between -1.2 radians and 0.3 radians and the reference of the rotation angle was chosen between 0 an 3 radians. We can observe that the control system behaviour is satisfactory in spite of significant changes.



Figure 9: Controlled signals (pitch and rotation angles) and appropriate reference changes (dashed lines)

CONCLUSION

Modelling and simulation is extremely important subject in all control engineering courses. Namely it is much easier, cheaper and safer to experiment in simulation environment as on real processes. However traditional block oriented causal approaches should be extended by more advanced object oriented acausal approaches and tools which are especially efficient in multi-domain applications.

In Karer and Zupančič 2006 the traditional modelling approach using causal traditional block diagram approach was used. In this paper however a more advances multi-domain and object oriented acausal modelling was used. There is no important difference

when modelling control schemes. However there is a big difference when modelling physical systems. The structure of the block diagram model in Matlab/Simulink does not reflect the topology of the physical system. It is not possible to transparently observe the stand, the helicopter body, the rotors, the revolute joints ... There is a fundamental limitation of block diagram modelling. The blocks have an unidirectional data flow from inputs to outputs. This is the reason why objects mentioned above cannot be dealt with directly. It is also the reason why some parameters of the different components appear in mixed expressions in the Matlab/Simulink model. And the developed structure can be more or less used only for the configuration it was developed. The effort to produce the Simulink simulation model is incomparable with the Modelica model. One needs much more time and much more modelling knowledge for Simulink based approach. There is no useful textual layer behind the diagram layer which is the important disadvantage of the Simulink model. So it is problematic to deal with complex and sophisticated models. The documentation is very difficult and inappropriate.

In Modelica models (Figs. 3, 4, 5), the connections between physical system and computer model are very transparent. All the components are fully reusable in other configurations. The combination of textual and diagram programming is efficient. So Modelica can be used for very complex problems and is also superior for model documentation.

We conclude that Matlab/Simulink is superior for the design and implementation of control schemes as it has more facilities especially in conjunction with some toolboxes – e.g. Control System Toolbox, Optimization Toolbox. Modelica is superior when modelling physical systems when the concept of algebraic manipulation and specially defined connectors bring many advantages. This approach is also very useful in education. We propose to start modelling courses with OO acausal approach especially when one can deal with implemented libraries which do not demand a deep theoretical background. And it can motivate students much more than the low level Simulink approach.

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Modeling and Simulation of Embryonic Hardware Structures Designed on FPGA-based Artificial Cell Network Topologies

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Abstract — The cell-based structure, which makes up the majority of biological organisms, involve nearly perfect selforganization, self-reproduction (multiplying), and faulttolerance properties in a well organized hierarchical mechanism. By adapting these mechanisms and capabilities from nature, scientific approaches have helped researches understand related phenomena and associated with principles to engine complex novel digital systems and improve their capability. Founded by these observations, the paper is focused on computer-aided modeling and simulation of embryonic hardware configurations designed on FPGA-based artificial cell network topologies. Own developed artificial cell model and artificial organism models are proposed, as basic components of a four level embryonic hardware structures. These models are careful tested through computer-aided investigations, using a specially developed software toolkit designed for VLSI systems real-time simulation operations.

I. INTRODUCTION

As well-known, the latest generations of VLSI (Very Large Scale Integrated) circuit's-based digital systems are characterized by highly computational and processing power, implemented on complex hardware architectures. Beside of its huge benefits in the control solutions implementation, unfortunately they introduce for designer engineers also a lot of difficulties booth in the fault detection and fault elimination operations [1], [2].

The solution from all these inconveniences seems to be offered by researchers from microelectronic sciences which have early discovered, that, by adopting selfhealing and surviving mechanisms of biological organisms from nature, becomes possible to design complex novel digital systems provided with highly faulttolerance and robustness properties. The basic idea is to imitate the biological organism's cell-based structure which involve nearly perfect self-organization, selfreproduction (multiplying), and fault-tolerance properties in a well organized hierarchical mechanism. Focusing on this strategy, it is expected to implement VLSI hardware structures able to simulate biological cells or artificial organism basic functions in similar mode with their equivalents from the living world [3], [4].

All these research efforts are based on a new concept born on digital systems design: the embryonic systems.

For this reason, basic concepts from cellular embryonic theory can be used for VLSI digital systems design. Therefore terms like artificial molecule, artificial cell and artificial organism are key concepts in developing and implementing embryonic hardware systems [5], [6].

II. EMBRYONIC SYSTEMS DEVELOPMENT STRATEGIES

The international research efforts in bio-inspired hardware systems (embryonic science) are very intensive and dynamic. This large interest is caused by the big problems in the more complex VLSI circuits manufacturing processes, which involve difficulties for designer engineers (manufacturing errors, circuits size, fault tolerance, etc.), and through the large impact in microelectronics informatics an technologies development (VLSI circuits minimization, nanotechnology scale circuits design and manufacturing).

At the international level, two basic models are developed for the bio-inspired digital embryonic systems: architecture with two-level embryonic structures, developed at University of York, England [1], [2], and architecture with four-level embryonic structures developed at the Swiss Federal Institute of Technology [3], [4].



Fig. 1. The four level of an embryonic system

Taking into account the differences between real world, biological and digital systems, the Logic Systems Laboratory from Swiss Federal Institute of Technology,

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EPFL Lausanne, developed a bio-inspired system architecture, founded on four level of organizing, similar to figure 1 [4], [5]. This is a POE-type (Phylogeny, Ontogeny and Epigenesis) embryonic system developed in analogy with the evolutionary processes of biological systems. In accordance with this model, these embryonic systems derive from the multi-cellular structure of complex living organisms with strong hierarchical organization from molecular to population levels. The POE classification was introduced at first time by the researcher E. Sanchez for the digital electronic systems classification [4]. It is important to note, that the only hardware model of the above mentioned POE-type systems is the basic located molecular level [4], [6].

A main conceptual difference regarding the classical POE-type embryonic structures implementation is expressed in figure 1, where is proposed a solution in which all 4 embryonic levels can be implemented as a novel digital FPGA (Field Programmable Gate Array).

III. FPGA-BASED ARTIFICIAL CELL MODEL FOR EMBRYONIC SYSTEMS DEVELOPMENT

Considering the observations made in the previous chapter, the paper presents some research efforts regarding the development of an FPGA-based artificial cell model with a generalized character, in order to reproduce with high fidelity the complex phenomena and interaction rules inside embryonic hardware systems. For this reason, an original structure for the artificial cell is proposed, as shown in figure 2. According to this model, each FPGA circuit is considered an artificial cell with 4 lattices capable of full operation in a network structure through specially defined data and control buses [7].



Fig. 2. Hardware model for FPGA-based artificial cell

Each lattice of the artificial cell has the same number of input/output bits and configuration structure, with the same operation functions. For example, the upper-lattice of the artificial cell has the following configuration:

- UI (*b0ui*, *b1ui*, *b2ui*, *b3ui*) - the data bus (4 input bits) to receive information from the upper neighbor cell;

- CkuI - the input data bus synchronization clock;

- UO (*b0uo*, *b1uo*, *b2uo*, *b3uo*) - the data bus (4 output bits) to send information to the upper neighbor cell;

- CkuO - the output data bus synchronization clock;

- AuI - signal received from the upper cell (alive=1, dead=0)/data transaction enable signal;

- AuO - the cell's internal signal (alive=1, dead=0)/data receive enable signal.

The same 12-bit configuration is used for the left, right, and down lattice of the artificial cell, and is specially designed for the full-operation of each FPGA circuit in a bi-dimensional artificial cell network [8].

Obviously, the proposed model is far not so complex; one artificial cell structure is suitable for convenient implementation also into one of the first generations Xilinx FPGA circuit. With the purpose to facilitate the operation algorithms for software implementation, the communication strategy between these cells is designed to work in a synchronous mode. It is wellknown, that now, the clock rate of several generation FPGA circuit's is up to 200MHz. In this case, a maximal rate of 1MHz is limited, with the purpose to avoid inherent electrical noises and perturbations in the cells via-bus communication process. Moreover, for convenient visual monitoring of the cells interoperation, it is recommended, in the first laboratory experiments, to decrease this communication clock rate nearly up to 50-100Hz.

With the purpose of facilitating the research and modeling process too, the artificial cells are organized in macro-groups of cell networks, each with 9 artificial cells, as it is presented in figure 3. In the software model indicated in this figure, each cell is an autonomous FPGA array, with special functions inside the organism, defined through an instruction set (program), and called the cell's gene. Each cell has a copy of all genes from the organism (operative genome), and depending on the cell's position inside the organism, only one cell has a gene operative (the cell's differentiation properties).



Fig.3. Model of artificial cell network (cluster)

In the presented model, the operative genome is designed with 5 genes (A, B, C, D, and E), and at the same time just one gene is shown active (highlighted in the figure). The cells which don't show any operative gene are considered spare cells (4 cells from the total of 9

in a cluster indicated in figure 3). It is important to note, that the implemented genes are generically labeled in the model with *A*, *B*, *C*, *D*, and *E*, but they can represent a wide range of control algorithms and programs (industrial process control, electrical motors control, etc.) defined by the software initialization process.

In accordance with the above mentioned strategy, in figure 4 an artificial organism model build with 4 macrogroup artificial cell network (clusters) is presented. In this model, a network with up to 40x40=1600 artificial cells is possible to be simulated. All cells in the artificial organism's structure are working according to the rules and communication abilities described in the FPGA-based model presented in chapter III.



Fig. 4. Model of the artificial organism

The artificial organism represents the 3rd level in the four level embryonic systems shown in figure 1 [9], [10].

IV. EMBRYONIC SYSTEMS COMPUTER-AIDED SIMULATION ENVIRONMENT

In actual stage of modeling and simulation software environments development, the international corporations offer two main categories of simulation toolkits for the electronic circuit designers:

- simulation environments were the signals (voltages and currents) are continuous in the real time domain (for example: OrCAD PSpice);
- simulation environments were the signals (voltages and currents) can have only Boolean values (for example: Electonics Workbench Digital environment).

Simulation with continuous variables in the time domain is almost difficult, because needs accurate and complex computations, and is not suitable far away for real-time simulation of digital circuits operation. The simulation with Boolean variables seem to be the most simplest, and is suitable even for real-time simulation of complex VLSI digital circuits. In such a case the simulation is made through by the elementary circuits from the environment's library (logic gates, flip-flops, counters, multiplexers, etc.), or using the high level hardware description languages developed for this reason (for example: VHDL for ASIC's, FGPA's, etc.). But usually these kinds of environments are developed for simulation of one VLSI circuit, as the main part of the designed electronic circuit.

In special cases where is necessary the complex digital systems simulation, with several VLSI circuits in a network, these environments also becomes difficult an inefficient for utilization, especially for real-time simulation expectations.

Taking into account the above mentioned observations is not very difficult to deduce the following conclusion: for the embryonic models and FPGA-based artificial network structures presented in the previous paragraph, is not available in the market an adequate software simulation toolkit. This conclusion lead the team involved in the above mentioned embryonic hardware structures development to design a new simulation environment, specially conceived for complex VLSI circuit's network topologies real-time simulation. The main window of this simulation software toolkit is presented in figure 5.



Fig. 5. Main window of the VLSI circuit's simulation software toolkit

The new simulation environment was conceived with a user-friendly interface, which allows the easy utilization and manipulation of the whole program. Figure 5 shows also the design pad where are pulled down the VLSI circuit's network. In accordance with the designer's expectations, de environment is able for real-time simulation of maximum 62500 digital circuits each with 8 pins, or a network with 25 VLSI circuits each own with maximum 400 pins. Of course, the hardware architecture of one complex circuit with 400 pins is implemented through VHDL language programming. In this reason, any kind of complex hardware can easily simulate in realtime operation, this depending only by the programmer's experience and its own implementation abilities.

To prove the new software toolkit generous simulation resources, in figure 6 a complex VLSI circuit's network is implemented on a design pad and prepared for real-time investigations.

External_Device1	Cluster1_1_Cell1_1	Cluster1_1_Cell1_2	Cluster1_1_Cell1_3
PIC 18F4550	FPGA_1_1	FPGA_1_2	FPGA_1_3
Keyboard	Cluster1_1_Cell2_1	Cluster1_1_Cell2_2	Cluster1_1_Cell2_3
	FPGA_2_1	FPGA_2_2	FPGA_2_3
	Cluster1_1_Cell3_1	Cluster1_1_Cell3_2	Cluster1_1_Cell3_3
	FPGA_3_1	FPGA_3_2	FPGA_3_3

Fig. 6. Simulation model of the FPGA circuit's based artificial cell network organized in one cluster

The figure shows an artificial cell cluster, according to the software model presented in figure 3. Each cell from this network is an FPGA-based circuit, with the operation mode, external buses and hardware structure proposed in the artificial cell model from figure 2. Beside this all, the whole network is initialized and programmed through by a PIC 18F4550-type general purpose microcontroller via personal computer.

The whole software simulation package is divided into three main components: the unit for the VLSI circuit's edition and modeling, the module for the real-time simulation, and more one unit for the graphical elements simulation created by the user. Of course, a user-friendly software oscilloscope included into the toolkit is also available, for convenient real-time monitoring of the followed digital signals in the given embryonic system.

V. COMUTER-AIDED SIMULATION RESULTS AND COMMUNICATION MONITORING

Considering, that the FPGA circuit's based artificial cells communicate with each other via instructions in the network, defined through the communication strategy and rules described and explained in detail as follows in [7], at first, the artificial structure presented in figure 7 was considered for investigations and real-time simulations.

The basic goal of these simulations is to evidence the important facilities offered through by the new software environment, to demonstrate the versatility of programming in high level languages the operation mode of complex VLSI circuits, as it was proposed in the FPGA hardware model indicated in figure 2. Not at least, in the given case, to prove the right communication path inside of one artificial cell network (or cluster).

In this case, for more convenience an *External Device* able to generate excitation signals for the cell cluster is also connected in the structure. For example, it is used to send an instruction to *Cell3_3* located in the right-down position of the cluster (with active gene *E*).



Fig. 7. Externally excited artificial cell network (example 1)

The obtained results can be followed in the timediagram presented figure 8. At first, by the connected *External Device* the *ExtDevice.Clk_o* signal composed of 8 clocks (one instruction) is generated to the right-side cell (*Cell1_1*). This signal is received by *Cell1_1* and through the *Cell1_1.ckro* is transmitted toward to the neighbor *Cell1_2*. In the same way the instruction is propagated in the cluster from one cell to other (the propagation path is marked through arrows). The *Cell3_3* computes a result for the external device using gene *E*, and at last *Cell1_1* returns through *Cell1_1.cklo* this result to the *External Device*.

External Device1.Clk o	
External_Device1.Clk_i	
Cluster1_1_Cell1_1.ckli	
Cluster1_1_Cell1_1.ckro	
Cluster1_1_Cell1_2.ckli	
Cluster1_1_Cell1_2.ckro	
Cluster1_1_Cell1_3.ckli	
Cluster1_1_Cell1_3.ckdo	
Cluster1_1_Cell2_1.ckdi	
Cluster1_1_Cell2_1.ckuo	
Cluster1_1_Cell2_3.ckui	
Cluster1_1_Cell2_3.ckdo	
Cluster1_1_Cell3_1.ckri	
Cluster1_1_Cell3_1.ckuo	
Cluster1_1_Cell3_2.ckri	
Cluster1_1_Cell3_2.cklo	
Cluster1_1_Cell3_3.ckui	
Cluster1_1_Cell3_3.cklo	

Fig. 8. Network communication strategy inside the cluster (example 1)

The presented time-diagram evidences the delays of instructions between the artificial cells, and the right path of the communication. A new set of numerical simulation results can be obtained, if more complex embryonic system is proposed for computer-aided simulation and investigation.

In figure 9 is presented an artificial cell network structure (artificial organism) with the 36 artificial cells of 4 clusters. Now two *External Devices* are considered for the excitation signals generation: one in the upper-left side, and other in the down-left side of the network. Suppose that, they generate signals in the network as shows the two paths marked in the figure with arrows.



Fig. 9. Externally excited artificial cell network (example 2)



Fig. 10. Network communication strategy inside the cluster (example 2)

The obtained result is shown in the software oscilloscope from figure 10. Following the paths marked with arrows from figure 9 and the communication signals expressed in the left side of figure 10, the right way of communication between the cells can be deduced.

From this point, the complexity of the modeled VLSI circuits (limited in the software toolkit to 25 circuits, each with a maximum of 400 connection pins) and the implemented algorithms (communication rules, genes implementation, etc.) length depends only by the experience and implementation abilities of the user.

VI. CONCLUSIONS

In the paper artificial cell model and artificial organism models are proposed, as basic components of the four level POE-type embryonic structures. By adapting basic mechanisms and capabilities of living organisms from nature, is expected to engine complex novel digital systems and improve their capability, with the same robustness and fault-tolerance abilities like their biological equivalents.

Also a specially developed simulation software toolkit is presented; with the purpose of complex VLSI circuit's real-time simulation interconnected in network topologies. The proposed models were careful tested through careful computer-aided simulations.

The proposed models and artificial structures can be a support for future developments in bio-inspired hardware systems, in order to found the theoretical basis, the design models or development methods of this new science domain named the embryonic systems.

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THERMAL BRIDGES DINAMIC SIMULATION AND HEAT TRANSFER COEFFICIENT VALUE FOR SPECIFIC THERMAL BRIDGES

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KEYWORDS

Thermal bridges, buildings thermal phenomena simulations, heat transfer coefficient simulation.

ABSTRACT

A thermal bridge is a part of the building envelope where the otherwise uniform thermal resistance is significantly changed by:

Full or partial penetration of the building envelope by materials with a different thermal conductivity and/or
A change in thickness of the structure and/or

• A difference between internal and external areas, such

as occur at wall-floor-ceiling junctions.

INTRODUCTION

The study of heat transfer in buildings can be achieved by subdividing the structure into wall types (walls, windows, doors, floors and roofs), for which heat losses can be calculated separately. This kind of calculation is normally based on a one- dimensional model, i.e. assuming that the walls are homogeneous and are composed of a number of parallel layers for which the heat flow is perpendicular, as shown in Figure 1.

The heat transfer can be described for such a model, given some simplifications, by the thermal transmittance of the wall (the U-value). This value gives the heat loss through the building element per unit of inside to outside temperature difference and per unit of surface of the building element:

$$U = \left(\frac{1}{\alpha_e} + \sum \frac{d_i}{\lambda_i} + R_a + \frac{1}{\alpha_i}\right)^{-1} [W/m^2K]$$
(1)

The size of the heat transfer (= the heat loss transmission ϕ t) is then given by:





Figure 1. Heat transfer through homogeneous building elements

THERMAL EFFECTS SIMULATIONS DUE TO THERMAL BRIDGES AND DETERMINE THE THERMAL BRIDGES HEAT TRANSFER COEFFICIENT

The thermal effects simulations due to the thermal bridges and the heat transfer coefficients were realized using the dedicated program for buildings thermal bridges simulation Heat 5.0

Thermal effects simulations due to thermal bridges and determine the thermal bridges heat transfer coefficient for an exterior wall without thermal insulation

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) The first analyzed structure is an exterior wall in contact with the exterior air and with the ground, without thermal insulation, the second analyzed structure is also for an exterior wall in contact with the exterior air and with the unheated floor basement, with thermal insulation. The considered thermal insulations are the expanded polystyrene and mineral wool.

In Figure 2 is presented the exterior wall without any thermal insulation. The exterior air temperature is $T_e=0^{\circ}C$, the ground temperature is $T_g=10^{\circ}C$, and the interior temperature T_i=20°C.



Figure 2. Exterior wall without thermal insulation - floor in contact with the ground, Heat 5.0

The right part of the figure indicates the component materials and the numbers on the figure indicates the wall component surfaces. The wall is made from concrete.

In tables 1 and 2 are presented the heat fluxes values for each part component of the wall and the limit conditions.

Table 1: Heat fluxes values for each part component of
the wall and the limit conditions

Wall surface	q[W/m²]	Q[W/m]	Length [m]	Limit conditions
3	1.2775	0.9581	0.75	[2] T=10
				R=0.13
4	0.6147	0.922	1.5	[2] T=10
				R=0.13
6	-0.1208	-0.1486	1.23	[3] T=0
				R=0.04
7	-0.2086	-1.7314	8.3	[3] T=0
				R=0.04
Heat transfer sum: 3.6E-5 W/m				
Heat transfer sum: 1.8801 W/m				

Table 2. Heat fluxes for each surface depending on the limit conditions

Heat transfer for each wall surface and the characteristics limits conditions			
Wall surface	q [W/m ²]	Limit conditions	

[2]	1.8801	[2]	(T=10 R=0.13)
[3]	-1.8801	[3]	(T=0 R=0.04)
Sum: 3.6E-5	5		

In the Figures 3 and 4 are presented the temperatures and heat fluxes variations due to the thermal bridges for the analyzed wall.



Figure 3: Temperatures variation for the analyzed wall



Figure 4: Heat fluxes simulation for the analyzed wall structure, Heat 5.0

Thermal effects simulations due to thermal bridges and determine the thermal bridges heat transfer coefficient for an exterior wall with thermal insulation

The Figure 5 presents the second wall section: the right part of the figure describes the component materials, so depending on the limitations zones the wall includes: 6 surface- expanded polystyrene, 3 and 4 surfaces: concrete, and the ground surface.



Figure 5: Exterior wall with polystyrene thermal insulation - floor in contact with the ground

without thermal insulation, Heat 5.0

Table 3 describes the heat fluxes and the limit conditions for the wall structure presented in the Figure 5.

Wall surface	q[W/m²]	Q[W/m]	Length [m]	Limit condition s	
3	2.1093	1.582	0.75	[2] T=1 R=0.13	
4	2.2503	3.3755	1.5	[2] T=1 R=0.13	
6	-0.0574	-0.0706	1.23	[3] T=0 R=0.04	
7	-0.3357	-2.7798	8.28	[3] T=0 R=0.04	
Unitary heat fluxes sum: 2.1071 W/m ²					
Total heat fluxes sum: 4.9575 W/m					

 Table 3. Heat fluxes values for each part component of the wall and the limit conditions

In the figures 6 and 7 are presented the temperatures and heat fluxes variations due to the thermal bridges for the wall described in the figure 5, exterior wall with polystyrene thermal insulation – floor in contact with the ground.

Figures 8 and 9 present the heat fluxes variations for different wall points of the structure depending on the wall thickness, for the wall structure without thermal insulation (figure 2).



Figure 6. Temperatures variations, Heat 5.0



Figure 7. Heat fluxes variations, Heat 5.0



Figure 8. Wall structure without thermal insulation heat fluxes variations in 3D, Heat 5.0,



Figure 9. Wall structure without thermal insulation heat fluxes variations depending on the wall

Figures 10 and 11 presents the temperatures variations depending on the wall thickness, in different point of the structure, for the wall structure without thermal insulation (figure 2).



Figure 10. Wall structure without thermal insulation temperatures variations in 3Dimensional domain, Heat 5.0



Figure 11. Wall structure without thermal insulation temperatures variations depending on the wall thickness, Heat 5.0



Figure 12. Wall structure with thermal insulation heat fluxes variations in 3D, Heat 5.0



Figure 13. Wall structure with thermal insulation temperatures variations depending on the wall thickness, Heat 5.0

Analyzing and comparing the two structures we can conclude: in the figures 8 and 12 are presents the heat fluxes variations for the two analyzed walls structures in three dimensional domains. For the first wall structure, wall without thermal insulation layer, the heat fluxes' had bigger values comparing to the second structure, the wall case that had thermal insulation layer (polystyrene), resulting that the heat loses for the first wall structure (figure 2) are higher comparing to the second wall structure (figure 5).

The figures 10 and 13 present the temperatures variations in three-dimensional domains for the two analyzed structures presented in the figures 2 and 5. We can observe that in the figure 12, the case of the second wall structure, wall with thermal insulation layer (figure 5) the temperatures are beginning to increase especially on the wall side were the thermal insulation is used, comparing to first wall, that had no thermal insulation, were the temperatures on the wall surface are almost equal to the exterior temperatures. Otherwise, the temperatures for the wall surface in contact with the ground are bigger because the ground temperature is considered 10 °C, and the exterior temperatures is 0°C resulting that the lowest temperatures of the wall structures are registered on the side in contact with the exterior air.

The structures were analyzes using the dedicated simulation program for determining the heat looses due to the thermal bridges influences, Heat 5.0.

THE HEAT LOOSES THERMAL COEFFICIENT DUE TO THE THERMAL BRIDGES EFFECT CALCULATION

The heat looses thermal coefficient due to the thermal bridges effect can be calculated using the formula (3) [DIN EN ISO 10211]:

$$\Psi_{a} = \frac{Q_{2D} - A_{1} \cdot U_{1} \cdot \Delta T + Q_{2D} - A_{2} \cdot U_{2} \cdot \Delta T}{1} \cdot \Delta T_{max(1,2)}$$
 [W/mK](3)

where:

 l_1 , l_2 – the lengths for the considered structures, [m];

 U_1 , U_2 – the two regions thermal transmitances, $[W/m^2K]$;

 $Q_{\rm 2D}$ – thermal flux calculated in the bi dimensional domain, [W];

 A_1 , A_2 – the surfaces aria, $[m^2]$.

 ΔT – temperature difference between interior and exterior air, [K];

l-structure length, [m].

 $\Delta T_{max(1,2)}$ – maximum temperature difference between the two considered regions, [K];

 ψ_{a^-} the thermal coefficient due to the thermal bridges effects, [W/mK].

For the two considered structures we will determine the thermal looses coefficients due to the thermal bridges effect.

The table 4 and 5 present the heat looses coefficient due to the thermal bridges effects for the two analyses walls structures.

Table 4. The heat looses coefficient due to the thermal bridges effects for the exterior wall without thermal insulation

DETAIL: Exterior wall - basement floor without						
thermal insulation						
Surface	Temperature					
	[°C]					
interior	20					
exterior	0					
ground	10					
Real heat looses	U Value	Surface	ΔT	U _{reg}		
	[W/(m2K)]	[m ²]	[K]	[W/m]		
Exterior wall (Ureg.)	0.148	1	20	2.970		
Floor	0.219	1	10	2.129		
			Sum:	5.159		
Real value for heat looses	Heat flux					
	[W/m]					
Heat looses (HEAT 5.0)	15.6777					
Minimal temperature	19.4					

Te=0°C				
			Sum:	15.677
Thermal bridge heat looses coefficient	Thermal bridges coefficient Ψa			
	[W/(mK)]			
$\Psi_{PE,ext}$ = $\Psi_{walf} \frac{Q_{heat} Q_{regota}}{\Delta \Gamma}$	0.526			
Total value for the thermal bridges heat looses coefficient			Ψa:	0.526

In the next tables will be calculated the thermal transmittances for each component surface of the exterior wall with thermal insulation, depending on the component materials (tables 5, 6, and 7).

Table 5. Thermal transmittance calculation for the exterior wall surface in contact with the exterior air

	Exterior wall				
	Thermal				
	resistance				
	[m ² K/W]	0.13			
	interior		Thermal	Thickness	
	1/α _i		conductivity	d	
	exterior	0.04		[mm]	
	$1/\alpha_a$	0.04			
	Elements 1		λ		
1	Aired concre	ete	0.090	200	
2	Polystyrene expanded		0.035	150	
3	Plaster		0.350	20	
	U value:		0.148		
			$W/(m^2K)$		
			Thickness	37.0	

 Table 6. Thermal transmittance calculation for the floor

 basement in contact with the ground

Floor in contact with the ground					
	Thermal resistance [m ² K/W] interior 1/α _i	0.00	Thermal conductivity	Thickness d	
	exterior $1/\alpha_a$	0.04		[mm]	
	Elements1		λ		
1	Aired concre	ete	0.090	150	
2	Concrete		2.300	150	
3	Polystyrene expanded		0.035	200	
	I	I value:	0.134		
	(value.	W/(m ² K)		
	Thickness 50.0				

Table 7. The heat looses coefficient due to the thermal bridges effects for the exterior wall with thermal insulation, polystyrene

DETAIL: Exterio	r wall – baseme	nt floor w	vith the	ermal
insulation		-	-	-
Surface	Temperature			
	[°C]			
interior	20			
exterior	0			
ground	10			
Real heat looses	U value	Surface	ΔT	U _{reg}
	[W/(m2K)]	[m ²]	[K]	[W/m]
Exterior wall (Ureg.)	0.148	1	20	2.970
Floor	0.134	1	10	1.336
			Sum:	4.305
Real value for heat looses	Heat flux			
	[W/m]			
Heat looses (HEAT 5.0)	5.0359			
Minimal temperature Te=0°C	19.4			
			Sum:	5.0359
Thermal bridge heat looses coefficient	Thermal bridges coefficient Ѱа			
	[W/(mK)]			
$\Psi_{\text{PE,ext}} = \frac{Q_{\text{heat}} - Q_{\text{reg,total}}}{\Delta T}$	0.037			
Total value for t loose	he thermal bridges coefficient	ges heat	Ψa:	0.037

CONCLUSIONS

Taking into account the comparative analyze of those two walls structures it can be developed the next conclusions:

The inside and limit temperatures are lower for the wall structure that doesn't has a thermal insulation (figure 10) comparing to the wall structure that has thermal insulation on the exterior (figure 13).

Considering the wall structure that has polystyrene insulation in contact with the exterior air, the heat looses coefficient due to the thermal bridges is $\Psi_a = 0.037$ W/mK, comparing with the wall structure that doesn't has thermal insulation $\Psi_a=0.526$ W/mK.

For the wall structure that doesn't has polystyrene insulation in contact with the exterior air, the thermal transmittance is U=0.148 W/m²K and for the structure in contact with the floor basement is, U=0.219W/m²K.

The wall structure that has polystyrene insulation in contact with the exterior air the thermal transmittance is U=0.148 W/m²K, and for the structure in contact with the floor basement is, U=0.134W/m²K.

The thermal transmittance for the surface of the wall in contact with the exterior air is bigger comparing to the surface in contact with the floor basement because the ground temperature is 10° C and the exterior air only 0° C, and both surfaces had thermal insulation, exterior wall had polystyrene expanded thermal insulation with a thickness of 150 cm comparing to the Floor in contact with the ground with a thickness of 200 cm.

Using the thermal insulation the heat fluxes variations will be lower and also the inside temperatures will grow up, especially if the thermal insulation is correct dimensioned and energetically efficient.

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INTELLIPave - CONSIDERING ASIDE FAILURE CRITERIA AND UNKNOWN VARIABLES IN EVOLUTIONARY INTELLIGENCE BASED MODELS FOR ASPHALT PAVEMENT

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KEYWORDS

Evolutionary Intelligence, Asphalt Pavement Modelling, Unknown Variables

ABSTRACT

On 2008 was published (Salini et al, 2008) the guidelines to use an artificial intelligence based approach to create high quality models to asphalt pavements, surpassing most of the well know problems and limitations of the current empiric and empiric-mechanistic approaches. This paper describe part of this new approach called INTELLIPave, with focus in show how to totally unknown variables are considered in the model in an implicit way, regardless its nature or complexity, and how the failure criteria is used aside, and no longer inside, of the model.

INTRODUCTION

Model the asphalt pavement are among the biggest challenges of the engineering. The consensus tell about an intrinsic viscous-elasto-plastic non-linear and anisotropic behaviour; very complex, but not sufficient to explain the performance, suggesting the existence of more undiscovered parcels of the behaviour or the inexistence of any kind of pattern. Aside of the intrinsic ones, the asphalt pavement behaviour is subject to the interference of many external factors, as the characteristics of the vehicles (speed, loads, *et cetera*) and the climate (temperatures, rainfall, *et cetera*).

Half of century ago a number of methods were developed for asphalt pavement design, but with almost no efforts to try model the asphalt pavement behaviour in a way allowing to include all or most of the variables. In general terms these methods are very simplistic and based on empiric or empiric-mechanistic approaches, with the performance represented by two or three empiric variables, like the ESAL (Equivalent Single Axle Loads), CBR (California Bearing Ratio) or the maximum strain in the asphalt concrete layer (Figure 01).

In the late 1990s was announced the development of a new method under the name AASHTO 2002 with the goal of solve most of the existing problems to asphalt pavement modeling and giving a new level of technical accuracy for the service life prediction; as its name suggests, this method was supposed to be finished in the year 2002. Many years after, in 2008, this remain as a promise, an utopia prisoner of a limitless net of problems due to its wrong paradigm: try to join in one single method the empiric philosophy, empiricmechanistic structural evaluation, a puzzle with many punctual studies and the results of the multimillion SHRP/SUPERPAVE program. Despite the time, efforts, labor and money used, until now it was not found a way to make it to work.

The current methods in use - empiric and empiricmechanistic - were in line with the technical-economic needs of the time when they were created, half century ago, but since that time the reality changed. Today the number of vehicles in the highways increased exponentially, and the vehicles are more and more heavy, shifting of a load capacity of 9 tons in the 1960s to over 80 tons in current days, and the construction and maintenance costs, for both materials and labor, increased many times. On the other hand environmental questions are also pressing the costs, due to restrictions, namely in mining materials like stone. And this conjunction occurs in a scenario where the available public funds for construction and maintenance of the highways are decreasing. These methods also do not provide any way to scientifically accumulate the knowledge, making hard for the pavement engineering

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use the experience of one highway into another as the experience remain empirically accumulated on the persons, and may be easily lost due to forgetting, retirement or death.

The lack of a scientific and high efficient methods for asphalt pavement modeling, including pavement design and management, are resulting in an deficient prediction of the asphalt pavement behavior, resulting in a premature failure and higher maintenance costs due the underdesign (University of Minnesota, 1999), or initial costs higher than the ideal due the overdesign, in both cases resulting in a poor cost-effectiveness, due to the available funds. The introduction and use of new and high performance materials may have also some impact (Brown S. F., 1978).

On the other hand, advanced techniques of evolutionary intelligence, including multi-valued extended logic programming, evolutionary computation and neural networks, are been used with great success to model problems with complex, disperse or uncertain behavior, allowing to bypass many limitations of the traditional approaches in handling large amounts of data. According to Salini et al (2008), the soft computing tools allow to model the asphalt pavement dilemma in a true and long waited scientific way, avoiding the subjectivity and well know limitations and problems of the empiric and empiric-mechanistic methods, once it handles all the variables without concessions or simplifications, creating a new paradigm for asphalt pavement modeling in line with the technical-economic needs of the XXI century.

This new approach is flexible, technologic intensive and allows for the gathering and accumulation of scientific knowledge. It is applied in three steps to a database containing the details for one full cycle of life time of the asphalt pavement history: (1) first, the data is evaluated in order to determinate the quality of the information available through the use of logic functions subjected to mathematical proof; (2) then, the database is optimized in order to determine the weight of every variable and piece of data, generating a model organized in the form of a matrix with billions of records; (3) finally, the matrix of data is used to train a set of neural networks which, once trained, will be able to do predictions for asphalt pavement design and management.

Among the innovations of this new approach are the spin-off of the failure criteria from the model and the consideration of unknown variables in an implicit way.

THE MODEL AND THE FAILURE CRITERIA

The current paradigm for asphalt pavements looks to explain the pavement performance using a failure criteria before model the behavior. For practical purposes, the failure criteria (like Strains; ε_t) is inside or part of the model (Figure 1). As no explanation for the behavior was found in half of century of tries, no good model was produced. In this new approach this problem is handled in a different way, the failure criteria is placed aside of the model, and no longer inside.

This is a very important paradigm change, because allow create very high quality models without the need for an explicit explanation of the behavior, but an implicit one, where the prediction will follow and reproduce the performance registered in a database. This new paradigm is not valid just for pavements, but also for any model for any kind of purpose.

For practical purposes the failure criteria will just point where the database will be "cutted", with the axles crossing the pavement below (after) that point eliminated because, according the criteria, the pavement is no longer serviceable.

This give a total flexibility to choose the failure criteria, because it can be evaluated according any kind of parameter, objective or subjective, technical, financial or even exotic or exoteric. The only must is to be able to indicate when the pavement no longer meet the chosen criteria, and cut the database in that point. The Figures 2, 3 and 4 show an example where the cracked area at 20% was chosen as failure criteria.

The pavement can be subject to many different deficiencies like cracking, rutting or roughness, and every one happens in a different time in the same asphalt pavement. This new approach allows the use of multiple criteria to design or manage the pavement, giving the possibility to forecasting different scenarios and to make better decisions.

For every criteria the database is cutted in a different point, the data need to be re-optimized and the neural networks, retrained.

MODELLING UNKNOWN VARIABLES IN AN IMPLICIT WAY

When the failure criteria is placed aside of the model, a new world of possibilities is open. One of the most interesting is in the fact of the used variables in the model assume another purpose: provide orientation about where the model can be used with accuracy, and for that are necessary a number of variables, but not ALL; the orientation need be good, but not perfect. In fact, the model can be constructed even without any variable, but in that case it will works almost at an empiric level.

When one variable is removed from the model is assumed that all the pavements evaluated or designed using the model will be subject of that variable in the exact same way the pavement used as source to the model was. The influence of the variable remains in the model, but in an implicit way, instead explicit. This logic is valid not just to the known variables, but also to all and any unknown variable; in another words, all unknown variables, regardless of its nature, complexity or relevance, are considered in the model in an implicit way.

The Figure 02 shows the model using the cracked area up to 20% as the failure criteria for the pavement service life when are used (symbolically) all known variables. The pavement is serviceable, with a cracked area equal or lower than 20%, up to the axle number 5667000.

The Figure 03 shows the same pavement, but with five variables eliminated. Again, the pavement remains serviceable up to 5667000 axles. One of the eliminated variables was the vehicle speeds, but its importance remains inside the model in an implicit way, because the pavement was subject of different speeds; the model just have no register about that speed. In this case the model can be used with accuracy to do predictions in highways where the expected speeds are in the same range of the speeds happened in the test section source of the data used to build the model.

In the Figure 04 are (symbolically) inserted all known and all <u>unknown</u> variables with influence in the pavement service life. As the failure criteria is aside of the variables, the end of the service life remain in the same position, with all unknown variables included in the model in an implicit way.

CONCLUSIONS

The failure criteria for the asphalt pavements can be successfully used aside of the model, instead inside, avoiding or solving most of the problems found in the empiric and empiric-mechanistic approaches. The split give a new world of possibilities to optimize the prediction system in order to improve the accuracy of the model, handling many or all variables at the same time, and making it flexible to be used any kind of criteria for failure, regardless of its nature, like technical, financial or other. All known and unknown variables can be considered in the model in an explicit or implicit way.

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ESAL = (shift factor) $\cdot (\varepsilon_t)^{-f1} \cdot (E)^{-f2}$

ESAL = Equivalent single axle loads (standard axle)

- $\boldsymbol{\varepsilon}_{\mathbf{t}}$ = Maximum strain
- E = Modulus
- f1, f2 = Adjusting factors
- shift factor = Laboratory-to-field adjusting factor

Figure 01 – Empiric-mechanistic Equation for Asphalt Pavement Service Life Prediction

Cracked area	%0	%0	%0	%0	%0	:	20%	20%	20%	21%	21%	21%	21%	:
	V4	74	1	a:			*	₹N	٧4	V4	4V	44	74	:
sles	V3	V3		re criteri	10% 10%		V3	V3	V3	V3	V3	V3	V3	:
Vehio	V2	٧2	: و ا			2	V2	٧2	V2	V2	V2	V2	V2	:
	٧1	٧1	٧1	٧1	٧1	:	٧1	٧1	٧1	۷1	٧1	٧1	٧1	:
	S6	S6	S6	S6	S6	:	S6	S6	S6	S6	S6	S6	S6	:
	S5	S5	S5	S5	S5	:	S5	S5	S5	S5	S5	S5	S5	:
esponse	S4	S4	S4	S4	S4	:	S4	S4	S4	S4	S4	S4	S4	:
Structural r	S3	S3	S3	S3	S3	:	S3	S3	S3	S3	S3	S3	S3	:
	8 8 8 8 8		S2	S2	S2	S2	S2	S2	S2	:				
	S1	S1	S1	; :	sed to e model		S1	S1	S1	S1	ated data	מוכם ממור	S1	:
	C7	C7	C7	י ל נ	Data u		C7	C7	C7	C7	Flimins		z C7	:
	6	9	٥	9			9	9	9	9	9	9	9	
	0	0	0	0	0	:	0		/	0	0	0	0	:
	C5	5 U F	the	iet	<u>व</u>			C5	C5	C5	C5	C5	C5	:
Climate	C4	C4	point of	se to me		:	C4	C4	C4	C4	C4	C4	C4	:
	C3	C3	Cutting	databa		:	C3	C3	C3	ß	C3	C3	C3	:
	C2	C2	C3	C2	5	:	C2	C2	C2	C2	C2	C2	C2	:
	C1	C1	C1	C1	C1	:	C1	C1	C1	C1	C1	C1	C1	:
Axles	-	2	с	4	5	:	5666998	5666999	5667000	5667001	5667002	5667003	5667004	:

ы С	п	Solar radiation	S1	П	Asphalt layer vertical strains	٧1	п	Tire type
8	п	Air temperature	S2	п	Asphalt layer pressures	V2	п	Vehicle speed
ខ	п	Rainfall	S3	п	Asphalt layer horizontal strains	V3	п	Vehicle weight by axle
2	п	Wind speed	S4	п	Moisture in the granular layer	V4	п	Vehicle class
C5	п	UV Radiation	S5	п	Granular layer pressures			
90 00	п	Groundwater level	S6	п	Granular layer strains			
C7	п	Pavement temperature						

Figure 02 – Pavement History – (Symbolically Representation for) All Known Variables

Cracked area	%0	%0	%0	%0	%0		20%	20%	 ✓ 20% 	21%	21%	21%	21%	
	V4	V4	<u>\</u>	ailure criteria:	racked area	p to zu%		V4	V4	V4	V4	V4	V4	:
Vehicles	V3	٧3	V3	∠3	: C	-	V3	٧3	٧3	V3	٧3	٧3	V3	:
	11	11	٧1	٧1	٧1	:	11	۲1	٧١	۲۱	11	11	٧1	:
	S6	S6	Se	SS	Se	:	S6	S6	S6	SS	S6	S6	S6	:
ural response.	S3	S3	S3	ß	ß	:	S3	S3	S3	ß	S3	S3	s3	:
Structural	S2	S2	S2	S?	ised to	he model	S2	S2	S2	S2		ated data	S2	:
Structu	1	1	-		Data used	uild ti							outortootootootoot	:
	S	S	S	۰. ک		ă	S1	7 S1	V S1	S1	, L		S,	
	C5 💧 S	C5 Z S	C5 S	C5 S'	C2		C5 S1	C5 7 731	C5 V S1	C5 🚺 S1	C5	C5	C5 S	
	C4 C5 A S	c4 c5 S	cof the c5 s	meet c5 s			CA C5 S1	C4 C5 V S1	C4 C5 V S1	C4 C5 🔨 S1	C4 C5	C4 C5	C4 C5 C5	
Climate	C3 C4 C5 S	c3 C4 C5 🚺 S	tting point of the C5 S	abase to meet C5 S			C3 C4 C5 S1	c3 c4 c5 7 51	C3 C4 C5 V S1	C3 C4 C5 🚺 S1	C3 C4 C5	C3 C4 C5	C3 C4 C5 S	
Climate	C2 C3 C4 C5 S	c2 c3 c4 c5 🚺 S	d Cutting point of the c5 S	database to meet c5 s	the failure criteria		C2 C3 C4 C5 S1	c2 c3 c4 c5 73	c2 c3 c4 c5 V S1	c2 c3 c4 c5 🔨 S1	C2 C3 C4 C5	C2 C3 C4 C5	C2 C3 C4 C5 S	
Climate	C1 C2 C3 C4 C5 AS	C1 C2 C3 C4 C5 C5 S	C1 Cutting point of the C5 S	C1 C1 C1 C5 C5	C1 C1 C1 C1 C1 C2 C1		C1 C2 C3 C4 C5 S1	C1 C2 C3 C4 C5 V3	C1 C2 C3 C4 55 V S1	C1 C2 C3 C4 C5 C3	C1 C2 C3 C4 C5	C1 C2 C3 C4 C5	C1 C2 C3 C4 C5 5	

Solar radiation	S1	п	Asphalt layer vertical strains	V1	п	Tire type
Air temperature	S2	п	Asphalt layer pressures	<u> </u>	I	Vehicle speed
Rainfall	S	11	Asphalt layer horizontal strains	V3	11	Vehicle weight by axle
Wind speed	2	I	Moisture in the granular layer	V4	п	Vehicle class
UV Radiation	85	ı	Granular laver pressures			
Groundwater level	S6	п	Granular layer strains			
Pavement temperature						

пппп

222228<mark>8</mark>8

Figure 03 - Pavement History – Eliminate Variables do not Change the Position Where the Pavement Stops to Meet the Failure Criteria

															1
Cracked area	%0	%0	%0	%0	%0	:	20%	20%	20%	21%	21%	21%	21%		
	۷n	۷n	۸N	۸n	٨N	:	۸n	/	٩	۲	۷n	۸N	۷n		
	:		:	ia:	-		V_{μ}	/:		- :	:	:	:		
ŝ	٧5	٧5	75	criter	area	%(Å	٧5	V5	٧5	٧5	75	٧5	:	
/ehicle	V4	V4	V 4	ilure	icked	to 20	44	V4	V4	44	V4	V4	V4	:	
-	V3	V3	K3	Fai	cra	dn	43	V3	V3	V3	V3	V3	V3	:	001
	٧2	٧2	V2	V2	V2	:	٧2	V2	V2	۲2	٧2	V2	٧2	:	Ě
	٧1	٧1	۲۱	7	۲۱	:	٧1	۲1	7	2	٧1	۲	٧1	:	
	Sn	Sn	Sn	Sn	Sn	:	Sn	Sn	Sn	Sn	Sn	Sn	Sn	:	I
	:	÷	÷	:	÷	:	:	:		:	:	:	:	:	111
	LS	LS	S7	S7	S7	:	LS	S7	S7	S7	LS	S7	LS		
ponse	S6	S6	S6	S6	S6	:	S6	S6	S6	S6	S6	S6	S6		
ural res	S5	S5	S5	S5	S5		S5	S5	S5	S5	S5	S5	S5	:	c
Structural	\$	\$	S2	22	S2	:	S4	S4	S4	S4	S4	S4	S4	:	niorto lo
	S3	S3	S3	S3	S3	:	S3	S3	S3	ß	S3	S3	S3	:	o porto
	S2	S2	S2	۶2	5		S2	S2	S2	S2	2	5	S2	:	
	S1	S1	S1	δ		nodel	S1	S1	S1	S1		ח חמומ	S1	:	ασγ
	Cn	Cn	Cn	ځ	a used	d the r	Cu	Cn	Cn	C	inoto		Cn		I
	÷		÷		Dati	ping	:			:	∼i ⊔		:		
	~						~				~	~			2
	ö	ö	ö	ö	ö	:	ö	ö	Ö	ö	ö	ö	ö	:	
	C7	C7	C7	C7	C7	:	C7	\mathbb{Z}	5	C7	C7	C7	C7	:	
nate	C6	с, В	of the	neet	 ella		ß	C6	C6	90 Ce	C6	C6	C6		
Clir	C5	C.5	point (e to n		:	C5	C5	C5	C5	C5	C5	C5	:	
	C4	77	utting	tabas feilu	e lallu	:	C4	C4	C4	C4	C4	C4	C4		c
	C3	5	ບ ເ	da t da	Š	:	C3	ខ	ខ	ខ	C3	ទ	C3		citoihor.
	C3	C2	3	C	3	:	C3	ß	ß	8	C3	ß	C3	:	5000
	C	C1	C	C	C	:	C	C	5	5	C	C	C	:	
Axles	٢	2	з	4	5	:	5666998	5666999	5667000	5667001	5667002	5667003	5667004	:	5

5	11	Solar radiation	S1	11	Asphalt layer vertical strains	٧1	II	Tire type
2	п	Air temperature	S2	п	Asphalt layer pressures	V2	п	Vehicle speed
ខ	11	Rainfall	S3	п	Asphalt layer horizontal strains	V3	11	Vehicle weight by axle
2	11	Wind speed	S4	п	Moisture in the granular layer	V4	11	Vehicle class
S	11	UV Radiation	S5	п	Granular layer pressures	V5	п	Unknown variable
80	11	Groundwater level	S6	п	Granular layer strains	۸N	п	Unknown variable "n"
C7	п	Pavement temperature	S7	п	Unknown variable			
8	н	Unknown variable	Sn	п	Unknown variable "n"			
ຽ	п	Unknown variable "n"						

Figure 04 - Pavement History – With the Consideration of All Known and Unknown Variables the End of the Service Life Remain in the Same Position

SEQUENTIAL ESTIMATION OF THE STEADY-STATE VARIANCE IN DISCRETE EVENT SIMULATION

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KEYWORDS

Steady-State Simulation, Variance Estimation, Sequential Output Analysis, Batch Means

ABSTRACT

For sequential output data analysis in non-terminating discrete-event simulation, we consider three methods of point and interval estimation of the steady-state variance. We assess their performance in the analysis of the output of queueing simulations by means of experimental coverage analysis. Over a range of models, estimating variances turns out to involve considerably more observations than estimating means. Thus, selecting estimators with good performance characteristics is even more important.

INTRODUCTION

The output sequence $\{x\} = x_1, x_2, \dots$ of a simulation program is usually regarded as the realisation of a stochastic process $\{X\} = X_1, X_2, \dots$ In the case of steady-state simulation, we assume this process to be stationary and ergodic.

Current analysis of output data from discrete event simulation focuses almost exclusively on the estimation of mean values. Thus, the literature on "variance estimation" mostly deals with the estimation of the *variance of the mean*, which is needed to construct a confidence interval of the estimated mean values.

In this paper, we are interested in finding point and interval estimates of the steady-state variance $\sigma^2 = \text{Var}[X_i]$ and the variance of the variance, from which we can construct confidence intervals for the variance estimates. Similar to the estimation of mean values, one problem in variance estimation is caused by the fact that output data from steadystate simulation are usually correlated.

The variance we estimate is not to be confused with the quantity $\sigma_0^2 = \lim_{n \to \infty} n \operatorname{Var}[\overline{X}(n)]$, sometimes referred to as *variance parameter* (Chen and Sargent, 1990) or *steady-state variance constant* (Steiger and Wilson, 2001),

and which is important in the methods of standardized time series (Schruben, 1983) and various methods using this concept.

Applications for the estimators we propose can be found in the performance analysis of communication networks. In audio or video streaming applications, for example, the actual packet delay is less important than the packet delay variation or jitter (see e.g. Tanenbaum, 2003). Other applications include estimation of safety stock or buffer sizes, and statistical process control.

Our estimation procedures are designed for sequential estimation. As more observations are generated, the estimates are continually updated, and simulation is stopped upon reaching the required precision.

In simulation practice, one observes an *initial transient* phase of the simulation output due to the initial conditions of the simulation program, which are usually not representative of its long-run behaviour. It is common practice to let the simulation "warm up" before collecting observations for analysis. For many processes, σ^2 converges to its steady-state value slower than the process mean; therefore, existing methods of detection of the initial transient period with regard to the mean value may sometimes not be applicable for variance estimation. A method based on distributions, which includes variance, is described in (Eickhoff et al., 2007). This is, however, not the focus of this paper, so we use a method described in (Pawlikowski, 1990).

In the next section we present three different methods of estimating the steady-state variance. We assessed these estimators experimentally in terms of the coverage of confidence intervals. The results of the experiments are presented in Section 3. The final section of the paper summarises our findings and gives an outlook on future research.

ESTIMATING THE STEADY-STATE VARIANCE

In the case of *independent and identically distributed* random variables, the well-known consistent estimate of the variance is

$$\hat{\sigma}^2(n) = s^2(n) = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x}(n))^2,$$
 (1)

and its variance is known to be (see e.g. Wilks, 1962, p. 200)

$$\operatorname{Var}[s^{2}(n)] = \frac{1}{n} \left(\mu_{4} - \frac{n-3}{n-1} \, \sigma^{4} \right), \tag{2}$$

where $\bar{x}(n) = \sum_{j=1}^{i} x_j/i$, is the sample mean of the first *n* observations, and μ_4 is the fourth central moment of the steady-state distribution.

In the case of *correlated observations* usually encountered in simulation output data, s^2 is no longer unbiased, but in fact (see Anderson, 1971, p. 448)

$$\mathbf{E}[s^{2}(n)] = \sigma^{2} \left(1 - 2 \, \frac{\sum_{j=1}^{n-1} (1 - j/n) \rho_{j}}{n-1} \right), \qquad (3)$$

where ρ_j is the lag j autocorrelation coefficient of the sequence $\{x\}$.

We propose three estimators of σ^2 : Method 1 treats it as a mean value and thus avoids dealing with the statistical problems associated with the estimate s^2 , Method 2 uses uncorrelated observations to overcome the bias problem of s^2 , and Method 3 compensates for this bias.

Method 1: Variance as a Mean Value

Variance is defined as the mean squared deviation of a random variable from its mean value: $Var[X] = E[(X - E[X])^2]$. This suggests that it should be possible to estimate variance as a mean value. We estimate the variance of a sequence $\{x\}$ as the mean of the new sequence $\{y\}$, defined by $y_i = (x_i - \bar{x}(i))^2$. This makes the point estimate

$$\hat{\sigma}_1^2(n) = \frac{1}{n} \sum_{i=1}^n y_i.$$

To obtain a confidence interval, any existing procedure of mean value estimation can be used. We use the method of spectral analysis, as proposed by (Heidelberger and Welch, 1981).

Method 2: Uncorrelated Observations

Processes typically encountered as simulation output data have a monotonically decreasing autocorrelation function; so, observations that are spaced "far apart" are less correlated, and if we choose a sufficiently large spacing, we can assume that the observations are (almost) uncorrelated. This enables us to use (1) as a point estimate of the variance.

We define a secondary sequence $\{y\}$ as $y_i = x_{k_0 i}$, where k_0 is the spacing distance needed to make the observations approximately uncorrelated. The ergodic property of the process $\{X\}$ ensures that $\operatorname{Var}[X_i] = \operatorname{Var}[Y_i] = \sigma^2$.

As point estimate we apply (1) to the sequence $\{y\}$:

$$\hat{\sigma}_2^2(n) = \frac{1}{m-1} \sum_{i=1}^m (y_i - \bar{y}(i))^2$$

where $m = \lfloor n/k_0 \rfloor$ is the length of the sequence $\{y\}$. To calculate the variance of the estimate, we use (2), replacing the actual values of σ^2 and μ_4 with their estimates:

$$\operatorname{Var}[\hat{\sigma}_{2}^{2}(n)] = \frac{1}{m} \left(\sum_{i=1}^{m} \left(y_{i} - \bar{y}(m) \right)^{4} - \frac{m-3}{m-1} \, \hat{\sigma}_{2}^{4}(n) \right)$$

The half-width of the confidence interval is then

$$\Delta_2 = z_{1-\alpha/2} \sqrt{\operatorname{Var}[\hat{\sigma}_2^2]}$$

We do not know of any general results on the distribution of $S^2(n)$; however, we can use a normal distribution because we assume the y_i to be uncorrelated, and their sample size to be large.

To find an appropriate value for the spacing k_0 , we successively test values by extracting the respective subsequences, and analysing their autocorrelation.

Method 3: Batch Means

We have seen in (3) that the sample variance of a finite, correlated sample is a biased estimate of σ^2 . When considering batches of observations of size m, we know that their means have a variance of (see Law and Kelton, 1991, p. 285)

$$\operatorname{Var}[\bar{x}(m)] = \frac{\sigma^2}{m} \left(1 + 2 \sum_{j=1}^{m-1} (1 - j/m) \rho_j \right).$$

Based on an unpublished paper by (Feldman et al., 1996), we show that adding $s^2(m)$ and $\operatorname{Var}[\bar{x}(m)]$ yields a consistent estimate of σ^2 . One can think of this as splitting the variance into two components, a *local variance* describing the short term variations of the process, and a *global variance* representing the long term variations. The local variance is calculated as the mean variance inside equal-sized batches, and the global variance is the variance of the means of the same batches.

To this end, we define a number of statistics: Given b equal-sized batches of size m, we calculate the sample mean and sample variance of each batch j, containing the observations $x_{j,1}, x_{j,2}, \ldots, x_{j,m}$ as

$$\bar{x}_{j} = \frac{1}{n} \sum_{k=1}^{n} x_{j,k}$$
$$s_{j}^{2} = \frac{1}{n} \sum_{k=1}^{n} (x_{j,k} - \bar{x}_{j})^{2}$$

Furthermore, we calculate

$$\bar{x} = \frac{1}{b} \sum_{j=1}^{b} \bar{x}_j$$

$$s_X^2 = \frac{1}{b-1} \sum_{j=1}^{b} (\bar{x}_j - \bar{x})^2$$

$$\bar{v} = \frac{1}{b} \sum_{j=1}^{b} s_j^2.$$

 \bar{x} and s_X^2 are the sample mean and sample variance of the batch means, and \bar{v} is the sample mean of the batch variances.

We now define the point estimator as

$$\hat{\sigma}_3^2 = \bar{v} + s_X^2.$$

We know that \bar{v} is an unbiased estimator of $E[S_j^2] = E[\frac{m-1}{m}S^2(m)]$, and that s_X^2 is an unbiased estimator of $Var[\overline{X}]$. So we can see that

$$\begin{split} \mathbf{E}[\hat{\sigma}_3^2] &= \mathbf{E}[\bar{v}] + \mathbf{E}[s_X^2] \\ &= \mathbf{E}[\frac{m-1}{m} S^2(m)] + \mathrm{Var}[\overline{X}] \\ &= \sigma^2, \end{split}$$

To obtain a confidence interval, we consider the statistic

$$y_j = s_j^2 + \frac{b}{b-1} \left(\bar{x}_j - \bar{\bar{x}} \right)^2$$

whose sample mean is equal to the point estimate $\hat{\sigma}_3^2$. Because we can express the variance estimate as the sample mean of a random sample, we can justify calculating the confidence interval using the sample variance of this sample:

$$s_Y^2 = \frac{1}{b-1} \sum_{j=1}^{b} (y_j - \hat{\sigma}^2)^2.$$

The half-width of the confidence interval is then

$$\Delta_3 = t_{b-1,1-\alpha/2} \sqrt{s_Y^2/b}.$$

Finding an appropriate batch size m is crucial in this estimator. If the batches are too small, the y_j will be correlated, and their sample variance s_Y^2 does not accurately describe the variance of the estimate $\hat{\sigma}_3^2$.

To determine the batch size we use a simple procedure which tests the first autocorrelation coefficients of the sequence of batch means, continually increasing the batch size until the correlation becomes negligible.

EXPERIMENTAL COVERAGE ANALYSIS

To assess the performance of the proposed estimators, we use the method of sequential coverage analysis, as described in (Pawlikowski et al., 1998). The estimators were

implemented using the Akaroa2 framework (Ewing et al., 1999).

We analyse the steady-state variance of the waiting times of customers in the single server queueing models M/M/1, M/E₂/1, and M/H₂/1. The model parameters are selected such that the coefficient of variation of the service time is 1 for the M/M/1 model, $\sqrt{0.5}$ for M/E₂/1, and $\sqrt{5}$ for M/H₂/1.

Simulations are run sequentially and stopped upon reaching a relative precision of 0.05 at the 0.95 confidence level. The coverage of confidence intervals is then calculated from the frequency with which the generated confidence interval covers the actual (theoretical) variance, and a confidence interval for the coverage is calculated at the 0.95 confidence level. Our procedure to analyse coverage follows the rules proposed in (Pawlikowski et al., 1998):

- 1. Coverage analysis is done sequentially.
- Our results include a minumum number of 200 "bad" confidence intervals.
- 3. Simulation runs shorter than the mean run length minus one standard deviation are discarded.

Each of the estimators is used on the three models at different system loads, ranging from 0.1 to 0.9. To deal with bias due to the initial transient period of the simulation we use the method described in (Pawlikowski, 1990), which is a combination of a heuristic and a statistical test for stationarity of the output sequence.

The Estimator $\hat{\sigma}_1^2$ (Figure 1) shows a coverage of around 0.93, which is slightly lower than the required 0.95, but still acceptable for most practical purposes. Because of its easy implementation (using an existing method of mean value estimation), this estimator can be interesting for practical use.

The estimator $\hat{\sigma}_2^2$ has generally good coverage (Figure 2), which shows that the method of "far apart" uncorrelated observations works.

Of the three estimators proposed, $\hat{\sigma}_3^2$ has the best coverage of confidence intervals (Figure 3).

In addition to the coverage of confidence intervals, we examine the convergence of the estimators on the basis of the number of observations needed to reach the required precision. Table 1 shows the mean number of observations collected before reaching that precision. Overall, Method 3 needs the fewest observation before the stopping criterion is satisfied, Method 2 needs the most. With increasing system load the simulation run lengths of all three estimators show a similar behaviour. It is worth noting that the run lengths in Table 1 are roughly an order of magnitude greater than those that would be required for estimating the mean waiting times to the same precision.

For the estimator $\hat{\sigma}_2^2$, we analyse the value of the parameter k_0 , which is automatically determined during the estimation process. Table 2 shows the average spacing used to produce almost independent observations. We see that the models with a higher coefficient of variation of the service



Figure 1: Coverage of Estimator $\hat{\sigma}_1^2$

Estimator $\hat{\sigma}_{2}^{2}$, M/H2/1 Queue

0.5 0.6 0.7 0.8 0.9

(c) M/H₂/1 Queue

0.4

0.98

0.94 0.95 0.96 0.97

0.92 0.93

0.1 0.2 0.3

Coverage

---- actual coverage ---- required coverage



(a) M/M/1 Queue





Figure 2: Coverage of Estimator $\hat{\sigma}_2^2$



Figure 3: Coverage of Estimator $\hat{\sigma}_3^2$

	M/	M/1 Qu	eue	M/	$E_2/1$ Qu	eue	M/	$H_2/1$ Que	eue
ρ	$\hat{\sigma}_1^2$	$\hat{\sigma}_2^2$	$\hat{\sigma}_3^2$	$\hat{\sigma}_1^2$	$\hat{\sigma}_2^2$	$\hat{\sigma}_3^2$	$\hat{\sigma}_1^2$	$\hat{\sigma}_2^2$	$\hat{\sigma}_3^2$
0.1	160	570	155	117	407	112	577	1736	552
0.2	131	365	123	94	265	89	556	1302	517
0.3	140	339	131	101	248	95	624	1291	567
0.4	172	372	158	125	275	118	752	1437	672
0.5	234	461	214	172	346	160	973	1744	862
0.6	359	652	325	266	494	245	1383	2342	1222
0.7	636	1078	571	481	826	435	2317	3646	2010
0.8	1491	2331	1322	1134	1776	996	5019	7282	4317
0.9	6237	9096	5509	5079	6942	4146	22044	26930	16750

Table 1: Mean Number of Observations Needed to Reach Required Precision (in 1000 Observations)

ρ	M/M/1	M/E ₂ /1	M/H ₂ /1
0.1	6.6	6.2	10.7
0.2	8.6	7.8	17.4
0.3	11.9	10.4	27.4
0.4	17.4	14.6	43.3
0.5	26.4	21.7	70.2
0.6	43.5	35.1	119.8
0.7	80.5	64.0	228.3
0.8	188.2	146.5	535.8
0.9	769.4	589.5	2213.5

Table 2: Mean Value of k_0 in Estimator $\hat{\sigma}_2^2$

time need larger values of k_0 due to the higher correlation of the output sequence.

CONCLUSIONS AND FUTURE WORK

In this paper, we introduced three different approaches for estimating the steady-state variance in discrete event simulation. We applied the estimators to single-server queueing models and compared them in terms of coverage and sample size needed to obtain confidence intervals of a certain precision.

So far, the proposed estimators have only been tested on single-server queues. Although we expect them to be applicable to a much broader range of models, further study is required to confirm this.

Methods 1 and 3 estimate the variance as the mean of a secondary sequence of observations. This suggests that the method of Multiple Replications in Parallel, as proposed in (Pawlikowski et al., 1994), can be used to speed up variance estimation by utilising multiple computers in parallel. While this is indeed confirmed by preliminary experiments reported in (Schmidt, 2008), further study is needed.

Method 2 has the obvious weakness of only using a fraction of the generated observations. Investigation is needed to determine if the method can be improved so that it does not discard as many observations.

Method 3 required the smallest number of observations and produced estimates with good coverage properties.

The sample sizes required for a certain precision turned out to be substantially larger than those needed to estimate comparable means, so selecting the best estimator is an important problem.

The problem of the initial transient period has not been addressed with regard to the steady-state variance. The method used in this paper (Pawlikowski, 1990) was designed for the estimation of mean values. Analysis of the warm-up period in estimation of steady-state variance is a subject of our future studies.

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ON NUMERICAL ESTIMATION OF PERFORMANCE ROBUSTNESS OF TRANSPORTATION NETWORKS

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ABSTRACT

The limited economic and spatial resources require a careful planning of investments, so that achieving the most accurate knowledge of the performances of any proposed solution is a problem of worth importance. A possible solution to this problem is provided by *sensitivity analysis* to evaluate their *robustness* to uncertainties. Then, in this paper, traffic simulations will be used to evaluate, by means of a proposed sensitivity analysis approach, the robustness of several interventions planned for the real case study consisting of the transportation network around the seaport of Genoa in Italy.

INTRODUCTION

In the last century, the continuous increase in traffic demand has been faced by firstly building new infrastructures and then, especially in the last two decades, by optimizing the performances of the already existing ones.

Therefore, it is well known that the limited economic and, especially in urban areas, spatial resources require a careful planning of investments, so that achieving the most accurate as possible knowledge of the performances of any proposed solution is a challenge to win. In this sense, the problem becomes more difficult whenever not only the present transport demand, but also the "estimated" future one, have to be taken into account.

Then, in this framework, most approaches for improving transportation network performances share the need of knowing, and often forecasting the traffic flows in the different links of the network itself. Despite this need, the problem of estimating traffic demand is difficult to be solved, especially when large and complex networks are taken into account, since traffic demand is affected by many sources of uncertainty. However, there are several different approaches for data acquisition, mainly characterized by different *temporal* and/or *spatial* levels of aggregation. In detail, from the temporal point of view, traffic data may be:

• *off-line estimated at once*, and eventually refined with periodical data sampling;

• *continuously acquired* by means of sensors which count and/or classify vehicles.

On the other hand, from the spatial point of view, traffic data may be acquired

- *globally*, i.e., by means of carefully planned measures in the whole considered network, thus leading to an "expensive" Origin-Destination (OD) matrix definition;
- *locally*, i.e., considering only the vehicle flows in particular locations and trying to estimate the OD-matrix by means of (relatively) few samples.

Furthermore, data may be aggregated with respect to the kinds of users, transportation modes, and so on.

Therefore, while the kinds of data to be collected depend on the particular problem to be faced, normally it is not usually possible to achieve a perfect knowledge of the origin-destination demand, as shown in recently published paper concerning Origin/Destination (O/D) matrix estimation, such as in Lundgren and Peterson (2008) and in Nie and Zhang (2008).

In this framework, finding a procedure which helps to choose, among the different possible improvements and modifications, and under uncertain mobility demand, the best interventions that may be implemented within budget and spatial constraints, is an interesting problem to solve.

A possible solution to this problem is provided by *sensitivity analysis* (see, for instance, Saltelli et al. (2004) for a general view of the problem), which, for what concerns transportation problems, dates back to the eighties (see, for instance, Tobin and Friesz (1988)).Then, although many of the achieved results to be formidable analytic methodologies, it is often difficult to apply them to real cases. In effect, the performances of transportation networks depend on structural/technological elements and on their interactions with the traffic demand in a way frequently difficult to be analytically described, especially when large networks are considered. This is the reason why, in practice, simulation is typically used in designing transportation infrastructures and in planning transportation services, instead of analytical modelling.

Then, in this paper, traffic microsimulation will be used for providing traffic data for sensitivity analysis of

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a real case study consisting of the transportation network around the seaport of Genoa, in Italy. Note that, being the basic ideas concerning the considered sensitivity analysis approach already presented in Di Febbraro and Sacco (2008), the aim of the present paper is to test, by means of numerical computations, the goodness of the methodology.

SENSITIVITY ANALYSIS

In the following sections, after giving a suitable definition of urban transportation network, the basics of the considered sensitivity indices are introduced.

Main definitions

The definition of *Urban Transportation Network (UTN)* here given has the aim of pointing out the interaction between the capacity of the infrastructures and the mobility demand. Then, for completeness of the description, the proposed approach, in the given definition the civil structures (roads, intersections, etc.), and the technological devices (such as traffic light controllers, Variable Message Signs (VMS), etc.) are considered separately.

Definition 1 Urban Transport Network

An UTN is the 4-uple

$$UTN = \{ \mathcal{C}, \mathcal{I}, \mathcal{K}, \mathcal{M}_{\mathcal{OD}} \}$$
(1)

where $C = \{C_j, j = 1, ..., J_C\}$ is the set of the centroids representing the different zones of the considered area, whereas $\mathcal{I} = \{I_j, j = 1, ..., J_I\}$ and $\mathcal{K} = \{K_j, j = 1, ..., J_K\}$ are the set of the civil infrastructures and of technological devices "working" in the considered area, respectively. Finally, the term $\mathcal{M}_{\mathcal{OD}} \in \mathbb{R}^{J_C, J_C}$ is the Origin/Destination (O/D) matrix, whose generic element $\mathcal{M}_{\mathcal{OD}}(i, j)$ is a non-negative real number representing the mobility demand from the centroid *i* towards the centroid *j*. In this definition, the elements representing the mobility demand with origin and destination in the same centroid are neglected, that is $\mathcal{M}_{\mathcal{OD}}(j, j) = 0, \forall j = 1, ..., J_C$.

Note that the above definition gathers both the *structural* and *technological* elements of a general urban traffic network, together with the relevant mobility demand.

Then, consider a set of m different network improvements which may be applied to an UTN. As said, these changes may be adopted in both the elements defining the transportation supply or network capacity, and may consist, for instance, of the introduction of new traffic controllers, or of the modification of the viability and the mobility demand, perhaps due to the modal shift towards public or railway transportation. Afterwards, given m different possible improvements, then there are $M_c = 2^m$ possible configurations, in which one or more of the improvements are implemented at a time. Then, it is possible to define the vector of all the possible configurations as follows.

Definition 2 Configuration Vector

The vector of all the possible configuration is defined as

$$s = \left[\begin{array}{ccc} s_1 & s_2 & \dots & s_{M_c} \end{array} \right] \tag{2}$$

in which each element is a sequence

$$s_i = \{s_i(k), \, k = 1, \dots, m\},$$
(3)

whose k^{th} element $s_i(k)$ is set to 1 (that is, $s_i(k) = 1$) or to 0 (that is, $s_i(k) = 0$), whether the k^{th} possible intervention is considered or not in the i^{th} configuration, respectively.

From the above definition, it results that the sequences

$$s_1 = \overbrace{\{0 \dots 0\}}^m$$
, and $s_{M_c} = \overbrace{\{1 \dots 1\}}^m$, (4)

represent the present network without any intervention and the configuration characterized by the presence of all the interventions, respectively.

For what concerns the O/D matrix, it is useful to define an Origin-Destination vector (OD-vector) as follows.

Definition 3 Origin-Destination vector

Let J_C be the number of centroids in the considered UTN, and assume that the couples with the same origin and destination centroid, that is those corresponding to the diagonal elements $\mathcal{M}_{\mathcal{OD}}(j,j) = 0$, are not considered. Then, the OD-vector is defined as

 $OD = \begin{bmatrix} od_1 & od_2 & \dots & od_{n_{OD}} \end{bmatrix},$ (5)

gathering the $n_{OD} = J_C(J_C - 1)$ demand elements od_j , $j = 1, \ldots, J_C$, corresponding to the non null elements of \mathcal{M}_{OD} .

Note that while some changes in an UTN may lead to the rising or the suppression of centroids, in this paper, for the sake of simplicity, the number of centroids J_C is considered to be constant. Nevertheless, such an assumption does not imply that mobility demand is also constant, since the elements of the OD vector can vary.

Performance index definition

Consider now the problem of evaluating the performances of an UTN for all the possible configurations in *s*. To this end, it is possible to define the following *performance index*, which explicitly depends both on the configurations and the mobility demand.

Definition 4 Performance vector

Let $\phi : s \times OD \to \mathbb{R}$ be a generic traffic performance function. Then, the performance vector is defined as

$$\Phi(s,OD) = \left[\phi(s_1,OD) \dots \phi(s_{M_c},OD) \right], \quad (6)$$

which gathers all the values assumed by the performance parameter $\phi(s_i, OD)$, which is computed for all the possible configurations, and by assuming the demand gathered in the vector OD. By this definition, the performance vector $\Phi(s, OD)$ results to have the same number of elements of the configuration vector s. Once computed the above vector, it is easy to determine the best UTN configuration i^* , since, depending of the chosen performance index, it is the one corresponding to the minimum or to the maximum element of the vector (6), that is

$$i^* = \arg\left[\min_{i=1,\dots,M_c} \phi(s_i, OD)\right],\tag{7}$$

or

$$i^* = \arg \left[\max_{i=1,\dots,M_c} \phi(s_i, OD) \right],$$
 (8)

respectively.

For instance, if the performance index ϕ gives the mean travel time in the UTN, then the best configuration is given by (7). On the other hand, if ϕ represents the mean vehicle speed, then the best configuration is given by (8).

Note that the performances parameter ϕ may be a suitable combination of different indices, thus taking into account, at a time, various aspects of the traffic problem, such as the mean travel time, the delay time, some pollution indices, the intervention building cost, a suitably defined cost-benefit ratio, and so on.

Definition of Sensitivity

Let consider the robustness of the traffic performances. As said, the elements of the vector OD are affected by uncertainties so that the *confidence* of the results in the vector $\Phi(s, OD)$ have to be carefully evaluated.

In order to cope with this problem, each element $\phi(s_i, OD)$ of the performance vector $\Phi(s, OD)$ may be associated to a set of *sensitivity measures* evaluated with respect of the demand od_j , $j = 1, \ldots, J_C$, uncertainty. Such indices are defined as the ratios

$$S_{\Phi}(i,j) = \frac{\frac{\partial \phi(s_i, OD)}{\phi(s_i, OD)}}{\frac{\partial od_j}{od_j}},$$
(9)

 $i = 1, ..., M_c, j = 1, ..., n_{OD}$, which express, for each configuration s_i , the relative deviation of the performance index $\phi(s_i, OD)$ computed with respect to its nominal value, compared with the relative variation of the term od_j .

Note that, in order to compute such values, Eq. (9) may be written as

$$S_{\Phi}(i,j) = \frac{\partial \phi(s_i, OD)}{\partial od_j} \cdot \frac{od_j}{\phi(s_i, OD)},$$
(10)

 $i = 1, ..., M_c, j = 1, ..., n_{OD}$, where:

- the partial derivative expresses how *amplified* or *reduced* is the variation of the performances when the demand *od_j* varies;
- the term *od_j* is the *nominal demand* for which the network improvements are designed;

• the term $\phi(s_i, OD)$ is the nominal performance, that is, the network performances computed at the nominal demand with the configuration s_i .

Then, the above sensitivity indices may be gathered in the following compact representation.

Definition 5 Sensitivity Matrix

The matrix $S_{\Phi} \in \mathbb{R}^{M_c, n_{OD}}$, defined as

$$S_{\Phi} = \begin{bmatrix} S_{\Phi}(1,1) & \cdots & S_{\Phi}(1,n_{OD}) \\ \vdots & \ddots & \vdots \\ S_{\Phi}(M_c,1) & \cdots & S_{\Phi}(M_c,n_{OD}) \end{bmatrix}$$
(11)

and gathering all the sensitivity parameters, is said "sensitivity matrix".

Then, once computed the sensitivity matrix S_{Φ} , it is possible to choose the most robust configuration with respect to the uncertainty of OD. In fact, it corresponds to the row which fulfills the minimum matrix norm criterion, that is

$$i^* = \arg\left[\min_{i=1,\dots,M_c} ||S_{\Phi}(i,:)||_p\right], \quad p = 1, 2, \infty,$$
 (12)

where $S_{\Phi}(i,:)$ is "Matlab-like" notation indicating the i^{th} row of the sensitivity matrix S_{Φ} , while the subscript p indicates the chosen norm.

For what concerns the meaning of the different norms in (12), it is worth saying that

1. when $p = \infty$, the norm coincides with the greatest element of the argument vector, that is

$$||S_{\Phi}(i,:)||_{\infty} = \max_{j=1,\dots,n_{OD}} |S_{\Phi}(i,j)|$$
(13)

Such a norm may be used to put into evidence the most critical situation, but does not takes into account the overall performance of the net;

2. when p = 2, the norm coincides with the Euclidean norm

$$||S_{\Phi}(i,:)||_2 = \sqrt{\sum_{j=1}^{n_{OD}} [S_{\Phi}(i,j)]^2}.$$

In this case, due to the squared values, the greatest elements of the row *i* weight more than the smaller ones. In particular, the contribution of the elements in the interval (-1, 1) is reduced, while those in $(-\infty, -1)$ and $(1, +\infty)$ is amplified;

3. when p = 1, the norm is given by the relation

$$||S_{\Phi}(i,:)||_1 = \sum_{j=1}^{n_{OD}} |S_{\Phi}(i,j)|.$$

In this case, all the elements of the vector $S_{\Phi}(i,:)$ are taken into account without any amplification or attenuation. This norm is useful when distortions in the sensitivity matrix have to be avoided.



Figure 1: View of Genoa.

Although the above defined index $\Phi(s, OD)$ and the relevant sensitivity matrix S_{Φ} give useful information about the best configuration to choose, they cannot be often easily computed due to the lack of analytical traffic models capable to take into account all the UTN aspects. In order to tackle with this problem, in the following section a simple procedure to compute the elements of the sensitivity matrix by means of a simulation approach is described.

Computing the sensitivity elements

In order to compute the sensitivity values of Eq. (11), the derivative in Eq. (9) may be approximated with the incremental ratio

$$\frac{\partial \phi(s_i, OD)}{\partial od_j} \simeq \frac{\phi(s_i, OD + \Delta_j) - \phi(s_i, OD)}{\delta}, \quad (14)$$

where

is a vector in which all the elements are null, but the j^{th} one, that assumes a small value δ .

With this approximation, it is possible to estimate the values of ϕ in (s_i, OD) and $(s_i, OD + \Delta_j)$, $i = 1, \ldots, M_c$, $j = 1, \ldots, n_{OD}$, by means of simulation. Then, the number of operations necessary to compute all the elements of the sensitivity matrix is

$$\#_{op} = M_c (n_{OD} + 1)\nu, \tag{16}$$

where ν is the number of statistical independent simulations which guarantees a good confidence of each parameter ϕ (see, for instance Law and Kelton (1991), for further details).

CASE STUDY

In this section, the formerly proposed methodology is applied to a real case study consisting of a portion of the urban transportation network of the city of Genoa (North-West of Italy) around the seaport.

The Genoa seaport transportation network

The considered case study consists of the urban area pointed out in Fig.1, which essentially represents the "junction" among the three high populated areas into which Genoa is divided.

In effect, as depicted in Fig.1, it consists of the portion of the Genoan urban network shared, at a time, by the freight traffic flows traveling from (resp., towards) the seaport towards (resp., from) the highway gate and the private/public traffic flows traveling from (resp., towards) the east side of the city towards (resp., from) the west one.

The choice of such a case study is motivated by the following reasons:

- the considered network is heavily influenced by the demand of mobility of goods by means of trucks, which use part of infrastructure to reach the highway from the seaport gates and vice-versa;
- as said, the considered area is also interested by the mean flows coming from the west and the north sides of the city and aiming to reach the center or the east side, thus resulting heavily congested in the rush hours;
- 3. some interventions are planned for this area. They mainly consist of improving the capacity of roads and roundabouts.

Then, to the aim of evaluating the performances of the planned interventions, and the relevant robustness, the O/D matrices of private users (cars and motorcycles)



Figure 2: View of the transportation network around the Genoa seaport.

have been *estimated* by means of several measures, repeated for some days in different places of the network, and a suitable traffic simulation software. On the contrary, the freight O/D matrix has been estimated by means of interviews to the seaport operators. As a consequence, the O/D matrix of the private users resulted to have low uncertainty (less than 5%, since measures may be accurately taken and sufficiently repeated), while the freight demand is somewhat more uncertain.

Present configuration

Consider the present configuration of the chosen network depicted in Fig. 2. In such a figure, the main elements are:

- centroids representing seaport gates (A, B, C, D);
- centroids representing the origin/destination of the private/public vehicles flows traveling in the area (E, F, H, L);
- a centroid representing the highway gate (G);
- the main, and critical from the point of view of their capacity, roundabouts (roundabout I and roundabout II);
- the main roads, indicated by means of dashed lines;
- the highway ramp, indicated by means of a dashed/dotted line.

Alternative Configurations

For what concerns the interventions which may be implemented in the considered area, they consist in making the road widths uniform, where possible (this intervention is already planned and essentially consists of creating the second lane in the road nearest to the seaport gates), and in the two following interventions:

1. the redesign of roundabout I, aiming at avoiding the left turn of vehicles coming from west. After this intervention, such vehicles, which represent a relatively negligible portion (less than 10%) of the whole flow, have to reach their destinations by means of alternative paths;

2. the change of the "right to way" in roundabout II aiming at limiting the flows conflicts, and thus reducing the probability of traffic jams. Also in this case, some users have to choose alternative paths to reach their destinations.

Therefore, there are four admissible configurations for the considered case study:

- s_0 : the present configuration, without interventions;
- s_1 : in this configuration only roundabout I is modified;
- s_2 : in this configuration only roundabout II is modified;
- s_3 : in this configuration both roundabouts are modified;

Note that in configuration s_i , i = 1, 2, 3, also the road enlargement is considered to be implemented, whereas it is not considered in configuration s_0 .

Then, the problem is comparing the different configurations and evaluating whether the increased travel times of users are balanced by a significant benefit for the whole network.

Simulation model

Then, for what concerns the simulation model used to compute the performance index and the sensitivity index, it consists of the TSS Aimsun model reported in Fig. 3, where, for the sake of clearness, the map layer is not depicted.

Numerical results

In this section, some numerical results relevant to the rush hour between 8.00 a.m, and 9.00 a.m. are discussed. In doing so, since in the chosen area the main problem is due to the trucks traffic entering/exiting the seaport gates,



Figure 3: AIMSUN model of the transportation network in the considered area.

in the discussed analysis only the effects of the uncertainty of such a demand are considered. In doing so, the demand vector *OD* resulted to have only 20 elements, corresponding to the 20 following non zero elements of the truck origin-destination matrix:

Then, for what concerns the simulation results, they have been obtained by means of ν repeated simulation runs, thus reducing the effects of the stochastic variables of the model and helping to obtain a good estimate of real performance values $\phi(s_i, OD)$, $i = 1, \ldots, M_c$, hereafter indicated with the general compact notation θ_i .

Obviously, as said, simulations only allow to compute an estimate of the real parameters θ_i , just providing the sample mean

$$\hat{\theta}_i = \frac{1}{\nu} \sum_{h=1}^{\nu} \theta(h)_i, \quad i = 1, \dots, M_c,$$
 (17)

where $\theta(h)_i$ is the value of the considered parameter computed, for the configuration *i*, during the h^{th} simulation run.

Finally, to compare the different configurations, a measure of the "distance" of the real parameter θ_i from its estimate $\hat{\theta}_i$ has been obtained by computing the confidence interval I, which is defined as the interval including the real parameter θ_i with an assign probability $(1 - \alpha)$, that is

$$\mathbb{P}\{\theta_i \in I\} \ge 1 - \alpha. \tag{18}$$

With this formulation, the confidence interval is

$$I = [\hat{\theta}_i - t_{\alpha/2,\nu-1}\hat{\sigma}_{\theta_i}, \,\hat{\theta}_i + t_{\alpha/2,\nu-1}\hat{\sigma}_{\theta_i}], \qquad (19)$$

where $\hat{\sigma}_{\theta_i}$ is the sample standard deviation

$$\hat{\sigma}_{\theta_i} = \frac{1}{\nu(\nu-1)} \sqrt{\sum_{h=1}^{\nu} (\theta(h)_i - \hat{\theta})^2},$$
 (20)

 $i = 1, ..., M_c$, and $t_{\alpha/2,\nu-1}$ is the parameter of the t-Student distribution with confidence α and $\nu - 1$ degrees of freedom. In this case, chosen $\alpha = 0.05$, satisfactory results have been obtained with $\nu = 6$.

Then, in Tab. 1 the sample mean and the confidence interval, computed as above recalled, of some important traffic performance parameters are reported. Looking at such results, it is easy to note that configuration s_1 is unstable, being its sample standard deviation (with these values it is unrealistic to compute the confidence interval) very high. In effects, the simulations of such a configuration are characterized by frequent jams, as, however, confirmed by the real network behavior. For what concern the best configuration, s_1 looks to be the best one, being characterized by the best value of 4/5 of the chosen performance parameters. Nevertheless, looking at the confidence intervals in Tab. 1, it is possible to note that all the proposed solutions lead to almost the same benefit with respect to the present configuration.

On the other hand, the norms of the sensitivity matrix indicates that the more "robust" configuration is s_3 for 4/5 of the parameters. Such a result suggests to implement such a configuration, which guarantees the stablest improvement of the network performances, with respect to the freight traffic uncertainty.

Conclusions

In this paper, some numerical results relevant to the sensitivity analysis of different configurations of interventions on the traffic network around the seaport of Genoa has been presented. In doing so, the proposed sensitivity indices has been computed by means of traffic simulation. The obtained numerical results show that, although all the configurations of interventions give almost the same benefit to the whole network, one of them results to be more robust with respect to the uncertainty of freight mobility demand in the considered area. To conclude, such results point out the importance of having a tool, such as the one here proposed, for robustness analysis in transportation.

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	unstable	configuration			stable co	onfigurations		
		s_0		s_1		s_2		s_3
	Mean	Std. Dev.	Mean	h.l. (95%)	Mean	h.l. (95%)	Mean	h.l. (95%)
Delay Time (s/km)	302.16	239.52	39.49	1.64	40.68	2.75	40.88	2.17
Density (veh/km)	55.58	45.18	5.87	0.17	6.16	0.13	6.1	0.43
Flow (veh/h)	1497.2	1136.46	2768.6	57.57	2775	58.63	2752.8	164.43
Speed (km/h)	22.67	11.14	35.26	0.57	34.99	0.34	35.08	0.31
Stop Time (s/km)	292.89	245.47	23.89	2.2	24.97	2.35	25.46	2.25

Table 1: Mean values and standard deviation of the configuration performances.

Table 2: Norms of the sensitivity matrix.

		$ S_{\Phi} $	$ _1$	
	s_0	s_1	s_2	s_3
Delay Time (s/km)	13.86	2.4	2.38	2.02
Density (veh/km)	1.39	1.14	2.82	0.9
Flow (veh/h)	38.22	0.93	1.23	0.72
Speed (km/h)	0.3	0.45	0.57	0.37
Stop Time (s/km)	26.14	3.93	4.54	3.04
		$ S_{\Phi} $	$ _2$	
	s_0	s_1	s_2	s_3
Delay Time (s/km)	4.62	0.7	0.73	0.59
Density (veh/km)	0.41	0.35	1.66	0.27
Flow (veh/h)	11.98	0.29	0.34	0.21
Speed (km/h)	0.08	0.15	0.16	0.11
Stop Time (s/km)	8.61	1.11	1.24	0.89
		$ S_{\Phi} $	$ _{\infty}$	
	s_0	s_1	s_2	s_3
Delay Time (s/km)	2.72	0.42	0.37	0.3
Density (veh/km)	0.19	0.21	1.62	0.17
Flow (veh/h)	7.64	0.18	0.13	0.11
Speed (km/h)	0.05	0.08	0.07	0.05
Stop Time (s/km)	5.46	0.63	0.56	0.43

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ANN MODELING AND SIMULATION OF GAS DRYING BY ADSORPTION ON COMPOSITE MATERIALS

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KEYWORDS

Gas-drying, Gas-solid adsorption, Neural network, Silica gel.

ABSTRACT

An artificial neural network (ANN) modeling of gas drying by adsorption in fixed bed of composite materials is presented in this paper. The experimental investigations were carried out at two values of relative humidity and three values of air flow rate respectively. The experimental data were employed in the design of the feed forward neural networks for modeling the evolution in time of some adsorption parameters, such as adsorption rate, water concentration in the bed, water vapor concentration in air at the exit from the fixed bed, drying degree and rate respectively.

INTRODUCTION

Recent studies on the adsorption system approach mainly the development of advanced adsorbent materials that give improved adsorption capacity and higher mass and heat transfer rates (Aristov et al., 1996; Aristov at al., 2002; Dawoud and Aristov, 2003; Liu and Wang, 2003; Zhang et al., 2005; Zhang and Liu, 2007). of Comprehensive experimental studies the physicochemical properties and some application researches of the composite adsorbents have been reported by Aristov et al. (Aristov et al., 1996; Aristov at al., 2002; Dawoud and Aristov, 2003), Liu and Wang (Liu and Wang, 2003) and Zhang et al. (Zhang et al., 2005; Zhang and Liu, 2007). All their studies point out that the composite adsorbents present a higher adsorption capacity and can be regenerated at lower temperature values. However, conclusions on the feasibility of these materials for adsorption systems can only be drawn after dynamic analysis of the composite adsorbent behavior under real operating conditions of adsorption systems.

In the last few years, neural network have attracted more and more interest as predictive models due to they are able to approximate any continuous nonlinear functions (Park and Sandeberg, 1991; Wang et al., 1992), being applied widely in the process modeling and control. Thus, Babu and Ramakrishna (Babu and Ramakrishna, 2003) concluded that the artificial neural networks (ANNs) model gives better results than regression technique for predicting results (output) from adsorption database. Otherwise, ANNs offer some quite interesting possibilities for rapidly developing nonlinear process model. In addition, the main feature of the neural networks - the establishment of complex relationships between data through a learning process, with no need to propose any model to correlate the desired variables - makes this technique very useful in the modeling of processes where traditional mathematical modeling is difficult or impossible.

Therefore, in this work is presented an ANNs study of gas drying by adsorption in fixed bed of composite materials with porous matrix. The experimental investigations were carried out using *LiBr*-impregnated silica gel grains of different shapes, and air at different values of the flow rate and air moisture. The experimental data were employed in the design of the feed forward neural networks for modeling the evolution in time of some adsorption parameters, such as adsorption rate, water concentration of the bed, water vapor concentration in air at the exit from the fixed bed, drying degree and rate. Regression equations rendering the evolution in time of the same adsorption parameters were also proposed and analyzed.

OVERVIEW ON ANN

Neural networks were originally inspired as being models of the biological nervous system. Thus ANNs might store experiential knowledge and make it available for use. In predicting an input-output response, ANN is viewed as a "black box" due to its mathematics involved is difficult to comprehend but very simple to implement. In recent years, there has been a growing interest in the application of ANNs in chemical engineering (Flood and Kartam, 1994; Satish and Pydi Setty, 2005).

The most popular neural network architecture in engineering investigations is the multilayer perceptron (MLP).

First, the neural network is trained in order to calculate optimal values of the weights. When the number of data used for training is huge or the number of hidden nodes is large, the training may take a long time. Once the network is trained, it can be tested on a different set of data than that used for training. It is a good approach to divide the given input/output data into two parts: one part (about 70%) is used for training whereas the other part usually smaller is used for testing the neural network model. The testing data set is reserved to validate the trained network.

Training and testing of the networks were performed by means of the *NeuroSolutions* software,

using the *Marquardt* algorithm and cross validation. In the studied case, the neural network model was determined as having four neurons in input, one hidden layer with eight neurons and one output, *MLP* (4:8:1).

EXPERIMENTAL

In the experimental investigations was used a laboratory installation (Fig. 1) consisting in an adsorption column, a wetting air column, a fan and devices for measuring and controlling temperature and air flow rate.



Fig. 1. Experimental installation: 1 – adsorption column,
2 – heat exchanger, 3 – thermostat, 4 – air wetting chamber, 5 – ventilator fan, 6 – digital technical balance, 7 – rotameter, 8, 9 – digital thermometers, 10,
13, 14, 15, 16 – valves, 11, 12 – chambers for measuring air relative humidity at the entrance and relatively exit of the adsorbed column.

The investigations were carried out using two types of composite adsorbent materials obtained from spherical silica gel particles having a diameter of $2.57 \cdot 10^{-3}$ m by impregnation with *LiBr*. The two composite materials, *MCSS2* and *MCS2*, differ by their geometrical shape, *MCSS2* having a spherical shape, while *MCS2* a non-spherical shape. Experimental investigations were performed under atmospheric pressure at an initial value of air temperature of $38 \,^\circ C$, using wet air as gaseous phase at two values of the relative humidity: 60 and $85 \,^\circ$, and at several values of air flow rate: 0.3, 0.6 and $1.2 \, m^3 \, h^{-1}$.

The adsorption process was achieved in fixed granular bed of composite materials under dynamic regime. The geometrical parameters of the fixed adsorbent bed were 0.15 m in height and $2.95 \cdot 10^{-2} m$ in diameter.

RESULTS AND DISCUSSIONS

For modeling the adsorption process, the water concentration in the fixed bed, X, water concentration of air at the fixed bed exit, C, adsorption rate, v_a , drying degree, η_u , and drying rate, v_u , were considered as functions of type y = f (material, C^0 , M_v , t), where: materials used were MCSS2 or MCS2, C^0 - water vapor concentration of wet air at the entrance in the fixed bed,

 M_v - flow rate of the wet air and *t*- time of adsorption. These parameters are defined as follows:

$$X = \frac{\Delta m + m_0 \cdot x_0}{m_0 (1 - x_0)}$$
(1)

where: m_0 – mass of adsorbent bed at t = 0, kg; Δm – mass of water uptake of the bed, kg; x_0 – water mass ratio in adsorbent at t = 0;

$$v_a = \rho_v \frac{dX}{dt} \tag{2}$$

where: ρ_v – apparent density of packing, $kg \cdot m^{-3}$;

$$\eta_u = 1 - \frac{C}{C_0} \tag{3}$$

where: C_0 , C – water vapor concentration in gas phase at the entrance and respectively exit of the adsorbent bed, $kg \cdot m^{-3}$;

$$v_u = \frac{1}{M_v} \frac{dw}{dt} \tag{4}$$

where: w – water vapor quantity removed from air flux, kg.

Regression Analysis

Experimental data points corresponding to the above-mentioned variables were collected and processed. Based on the experimental data and using specialized software for curve fitting (Table Curve 2D, 5.01, trial version), a series of statistical equations defining X, C, v_a , η_u , v_u as functions of time were determined. In the selection of these equations, three criteria were followed: the accuracy in modeling the experimental data, the simplicity of the equations and the use of a single equation pattern for all the experimental data sets. Consequently, four order polynomials with different numerical coefficients were considered.

$$y = a + b \cdot t + c \cdot t^{2} + d \cdot t^{3} + e \cdot t^{4}$$
 (5)

where y = X, *C*, v_a , η_u , v_u , and *t* is the time, min.

Table 1 presents the numerical values of the coefficients in equation (5) of the adsorption parameters corresponding to $0.6 \text{ m}^3/\text{h}$ and 60 %RH.

Table 1. Some values of the coefficients in eq. (5).

Nr.	Dep.	Mat		C	Coefficier	nts	
Crt.	Var.	Iviat.	а	b	с	d	e
1	Х		4.8E-03	1.7E-03	-2.2E-06	-4.2E-08	1.9E-10
2	С	22	1.2E-03	-9.8E-06	3.7E-06	-3.8E-08	1.1E-10
3	v_a	ICS	2.2E-02	2.2E-04	-9.8E-06	9.9E-08	-3.4E-10
4	η_u	Σ	9.6E-01	3.4E-04	-1.3E-04	1.3E-06	-4.0E-09
5	v_u		4.6E-05	1.7E-08	-6.3E-09	6.5E-11	-2.0E-13
6	Х		5.0E-03	1.7E-03	5.0E-06	-1.2E-07	4.5E-10
7	С		2.6E-03	-2.1E-04	7.4E-06	-6.3E-08	1.8E-10
8	Va	ICS	2.0E-02	2.5E-04	-7.4E-06	5.4E-08	-1.2E-10
9	η_u	2	9.1E-01	7.3E-03	-2.6E-04	2.2E-06	-6.2E-09
10	v_u	-	4.2E-05	4.8E-07	-1.6E-08	1.4E-10	-4.3E-13

The obtained equations allow the determination of the adsorption dependent variables (X, C, v_a, η_u, v_u) at any moment in the time range investigated experimentally.

 Table 2. Statistical parameters of the suggested equations.

		Statistical	parameters	
Nr. Crt.	R ² Coef Det	Fit Std Err	F computed	F- distribution,
				$(\alpha = 0.05)$
1	0.99998	2.3765E-04	115589.45	4.75
2	0.99897	1.5746E-04	1689.92	4.96
3	0.99679	3.5095E-04	544.09	4.96
4	0.99897	5.4744E-03	1689.92	4.96
5	0.99968	1.4063E-07	4719.49	5.12
6	0.99632	5.1310E-05	474.01	4.75
7	0.99998	2.5968E-04	124886.05	4.96
8	0.99947	1.9873E-07	2848.64	4.96
9	0.99949	4.6569E-03	3405.93	4.96
10	0.99881	2.5826E-04	1471.41	5.12

As can be seen in Table 2, the values of the determination coefficient of equations are near unity, while standard error and maximum absolute error have very low values, which show four-order polynomial functions fit very well the experimental data. Moreover, F-computed >> F-distribution for $\alpha = 0.05$, which underlines that all the suggested equations are adequate.

Regression equations allow the determination of the adsorption parameters at any moment in the experimental time range. Working with these equations is not difficult, but the numerical coefficients for different conditions of the adsorption process are necessary. Compared to these empirical models, the neural network modeling presents the advantage of supplying rapidly and easily the parameter values.

Artificial Neural Network

The experimental data points corresponding to the above-mentioned variables were collected and processed. The four variables listed in the right-hand side of above equation were considered as input variables while the *X*, *C*, v_a , η_u and v_u were considered as the output values. Thus, each *ANN* presents four input variables and one output variable.

In the training phase, the statistical parameters: linear correlation coefficient (R), mean squared error (MSE) and mean absolute error (MAE) (Table 3) indicate that the neural models describe well the adsorption process.

In Fig. 2 is presented an example that shows a comparison between experimental data and neural network predictions on training data. A good agreement

is emphasized proving that the neural model has learned well the behavior of the studied process.

Table 3. Statistical characterization for training phase.

Variable	R	MSE	MAE
X(kg/kg)	0.99679	2.6574E-05	4.06677E-03
$C (\text{kg/m}^3)$	0.99707	2.0000E-07	3.3460 E-04
$v_a (\text{kg/m}^3 \text{s}^{-1})$	0.98820	2.0085E-08	1.1103 E-04
η_u	0.99829	3.2270E-13	3.9882E-07
$v_u(\text{ kg/m}^3\text{s}^{-1})$	0.99901	1.1403E-04	7.6367E-03
$v_u(\text{kg/m}^3\text{s}^{-1})$	0.99901	1.1403E-04	7.6367E-03



Fig. 2. ANN predictions versus experimental values for water concentration of *MCS2* at $C^0 = 0.02876 \text{ kg/m}^3$ and $M_v = 1.2 \text{ m}^3/h$.

The purpose of direct neural modeling lies in the obtaining the network (group of formula) describing the dependences between the experimental data defining the investigated process. The elaborated neural model was then applied for several sets of experimental data in order to generate the necessary outputs. For validation, there were used new data that were not employed in the network training. In the studied case, the network *MLP* (4:8:1) received inputs unemployed in the training process and generated output values. Several of the achieved results corresponding to MCSS2, 0.6 m³/h and 60 %RH are presented in Table 4.

Table 4. Statistical characterization for validation phase of MLP (4:8:1).

Nr. Crt.	Dep. Var.	t (min.)	Y exp	Y RNA	Rel. error (%)
1	X	10	2.144E-02	2.350E-02	9.61
2	С	30	3.421E-02	3.098E-03	9.42
3	v_a	50	2.026E-03	1.991E-03	1.72
4	η_u	60	6.407E-01	6.386E-01	0.32
5	v_u	50	2.514E-05	2.447E-05	2.67

The good results obtained in the validation stage allow the utilization of the neural model in order to perform predictions corresponding to other operating conditions than the experimental ones. In this way, there were considered both types of composite materials, the two values of C^0 (Table 4), air flow rate and time were varied from $0.1 m^3/h$ to $2 m^3/h$, respectively, from 0 to 120 min. with a 5 min. step. Thus, a high number of data were generated and employed in order to describe the adsorption process on the used composite material on a range wider than that experimentally investigated as presented in Figs. 3-5.

In Fig. 3 are shown the regression equations and neural network predictions for water concentration in MCSS2 materials as function of time, maintaining the same air moisture at the entrance of the fixed bed, at several values of the air flow rate.





As can be seen, water concentration in adsorbents increases in time, while increasing of air flow rate accelerates the adsorption process.

In Fig. 4 are described the variations in time of water vapor concentration of wet air at the exit from the fixed bed at several values of air moisture.



Fig. 4. Regression equations (a) respectively ANN predictions (b) (lines) and experimental data ($\mathbf{O} - C^0 = 0.02876 \text{ kg/m}^3$, $\star - C^0 = 0.04145 \text{ kg/m}^3$) for water vapor concentration of wet air at the exit from the fixed bed of MCS2, at $M_v = 0.6 \text{ m}^3/h$. In (b) $1 - C^0 = 0.021 \text{ kg/m}^3$; $2 - C^0 = 0.024 \text{ kg/m}^3$; $3 - C^0 = 0.02876 \text{ kg/m}^3$; $4 - C^0 = 0.0323 \text{ kg/m}^3$; $5 - C^0 = 0.037 \text{ kg/m}^3$ şi $6 - C^0 = 0.04145 \text{ kg/m}^3$.

Water vapor concentration of wet air at the exit from the fixed bed increases in time and at high values of air moisture. This is due to a higher driving force of adsorption process. On the contrary, the drying degree decreases in time and with lower values of air moisture.



Fig. 5. Regression equations (a) respectively ANN predictions (b) (lines) and experimental data ($\Box - M_v = 0,3 \ m^3/h$, $\bigcirc -M_v = 0,6 \ m^3/h$, $\bigtriangleup -M_v = 1,2 \ m^3/h$) for adsorption rate corresponding to MCSS2, at $C^0 = 0.02876 \ kg/m^3$. In (b): $1 - M_v = 0.1 \ m^3/h$; $2 - M_v = 0.3 \ m^3/$; $3 - M_v = 0.5 \ m^3/h$; $4 - M_v = 0.6 \ m^3/h$, $5 - M_v = 0.9 \ m^3/h$; $6 - M_v = 1.2 \ m^3/h$; $7 - M_v = 1.4 \ m^3/h$.

In Fig. 5 are depicted the time dependences of adsorption rate for MCSS2 composite material corresponding to several values of air flow rate.

Increasing air flow rate leads to higher adsorption rates, which is due to weaker resistances to the external mass transfer.

As it can be noted, the predicted curves are in very good agreement with the experimental data. The predicted data outside and inside the investigated range of experimental conditions respect the typical behavior of the investigated process.

Though the results of the empirical polynomial equations seem to be better than those of the neural models, one should have in mind that each equation is based on its own set of numerical coefficients, while the neural network weights are available for the entire experimental range. It can be concluded that the experimental data are well modeled by both empirical polynomial equations and neural networks. However, the empirical equations are difficult in handling, while the neural models are easy to built, have simple topologies and short training times.

CONCLUSIONS

This work presents two types of empirical models for gas drying by adsorption, namely, artificial neural networks and regression equations. These models render the evolution in time of the ratio of water to adsorbent material, X, water vapour concentration of wet air at the exit from the fixed bed, C, adsorption rate, v_a , drying degree, η_u , and drying rate, v_u .

Regression equations represented by forth-order polynomials were proposed to model the considered adsorption parameters. These equations were validated by the determination coefficients, and their adequacy was tested by using Fischer test. However, the fact that the numerical coefficients have to be changed for each set of experimental conditions represents a major drawback. In addition, for any new operating conditions outside the investigated domain, the numerical values of the coefficient are no longer valid.

The artificial neural network models were validated by two methods. Data predicted in the training phase were compared with the experimental data on which the training phase was based. The very good agreement between model and experimental data proved that the neural network learned well the behavior of the adsorption parameters. Moreover, the predictions of the neural networks were compared with another set of experimental data that were not employed in the training phase. Therefore, the suggested neural network can be easily used to interpolate and extrapolate data of the adsorption process investigated for different conditions.

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SYSTEM LEVEL MODELING, SIMULATION AND VERIFICATION OF A CAN PHYSICAL LAYER STAR NETWORK USING BEHAVIOR MODELING LANGUAGE

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KEYWORDS

CAN physical layer verification, CAN network system modeling and simulation, CAN star topology, Mentor Graphics System Visions, VHDL-AMS.

ABSTRACT

The star topology is sometimes used in automotive applications to overcome wiring constrains within a car. It has to be mentioned that star topology is neither covered by ISO11898 nor by SAE J2284 therefore it is recommended to prove the feasibility of a specific topology in each case by simulations or measurements on a system setup (NXP-Semiconductors 2006). This paper considers the verification of an 8-node CAN physical layer star network by using behavior modeling and simulation in comparison to measurement. The main purpose is to verify the CAN transceiver behavioral model together with other CAN physical layer simulation components against measurements at system level. The measurement environment of the CAN network modeling methodology is discussed, showing how to get the measurement and simulation results matched. This demonstrates that it is a reliable simulation solution, which is highly desirable and very important for the verification requirement in CAN physical layer design. Last but not least, the paper also shows that different network topologies at different transmission rates can also be simulated to gain better understand about the behavior of CAN network in the early phase of design process.

INTRODUCTION

Designers face challenges in implementing hardware of CAN network's architecture, topology, termination and interconnect. The main task in analyzing physical layer is to identify and evaluate signal integrity issues for the network (Synopsys 2007). The transmitted and received waveforms need to be checked against system specification. Problems which relate to the physical layer will impact the entire communication system, slow down the network performance or cause errors in the control system behavior. Moreover, in-vehicles networks nowadays also have a very high complexity

due to the increasing number of ECU and functionalities. From an analysis of almost 100 different topologies of auto makers all over the world, more than 50% of these design failed when all the parameters involved had been in their worst-case conditions (Lawrenz and Bollati 2007). Therefore, there is a very great demand in verifying such critical designs.

Almost all car manufacturers and semiconductor suppliers have started simulations based on different modeling activities as a part of their development and verification process (Thorsten and Carsten 2005), (Pelz et al. 2004), (William et al. 2007), (Ravatin et al. 2002). They tried to simulate the in-vehicle network with different types of models (e.g. VHDL-AMS models, MAST models). However it is still not clear how much one can rely on simulation because putting the simulation models together and simulating those do not necessarily mean that simulation will reflect the physical system.

Improving CAN network reliability and quality requires a comprehensive and reliable simulation environment to manage complex communication network issues. A reliable simulation solution means that simulation should resemble real situation by at least 80%. In order to achieve a reliable simulation solution, simulation models need to be verified for its accuracy against the physical models. Several verification techniques are discussed in (Pelz 2003), however, these techniques concentrate on verification of the simulation models at conceptual level. One of the disadvantages in these techniques is that although the verification process is carried out at each the individual models, putting them together do not mean the simulation system will reflect the same as in reality. This paper aims to simulate all of CAN physical layer components in the context of system level, which means that not only the transceivers, chokes, transmission lines are simulated but the measurement environment of the CAN network is also taken into account. This is also a key for the matching between measurement and simulation.

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Components of CAN physical layer

The CAN physical layer presented in this work involves the following main parts:

- CAN Transceivers
- Choke coils are placed between the transceiver and the bus line to harmonize non-symmetric differential mode signals
- CAN bus line/ Twisted-pair transmission line
- Termination circuits are typically attached to the end to transmission line to reduce reflection on the CAN Bus

Nominal voltage level on the CAN bus

Figure 1 shows the nominal voltage level on a CAN bus when it operates ideally. A bus node shall detect a recessive bus condition (bit '1' is transmitted) when the voltage difference between CAN_H and CAN_L is not higher than 0.5V. The bus dominant condition (bit '0' is transmitted) shall be detected if the voltage difference between CAN_H and CAN_L is more than 0.9 V. When the bus operates at recessive mode, both CAN_H and CAN_L have 2.5V amplitude, while it is 3.5V for CAN_H and 1.5V for CAN_L when the bus operates at dominant mode.



Figure 1: Nominal voltage level on CAN bus

THE SYSTEM MEASUREMENT SETUP

For demonstration, a full CAN network is developed for measurement. The measurement CAN network consists of 8 nodes connected in star topology with different stub lengths as shown in Figure 2. A split termination circuit (2x62Ohm and 1x47nF) is implemented at the star connection point. At every node, the new choke coil founded in (Nguyen et al. 2008) with higher coupling factor between the two wires in the coil, is used to effectively reduce ringing on the CAN network.



Figure 2: The 8-node star CAN network with different stub lengths configuration

The whole CAN measurement setup with measurement equipments is shown in Figure 3.



Figure 3: The 8-node CAN measurement system

A CAN triggering module from LeCroy, which will be explained in more details, is used together with the oscilloscope for the measurement of CANHi and CANLo signals.

MODELLING OF THE CAN PHYSICAL LAYER COMPONENTS

System Vision simulation environment

All of the components of the 8-node CAN physical layer network were modeled with VHDL-AMS and simulated in System Vision simulation environment. System Vision is a virtual lab for creating and analyzing analog, digital, and mixed-signal system. Schematics/Designs can be created via schematic entry. System Vision provides a variety of simulation types from basic such as transient (time domain) or AC (small signal) analysis to advance such as Monte Carlo or parameters sensitivity analysis. Description of simulation models is discussed in the following sections.

Transceiver simulation model

Signal integrity of the CAN network is fundamentally impacted by transceiver (Thorsten and Carsten 2005). Therefore the transceiver model must be very accurate. A model of the CAN transceiver, developed by Infineon Technologies AG, is used. It was specially modeled for system simulation using VHDL-AMS because of simulation speed and accuracy reasons.

Figure 4 shows a block diagram of the Infineon CAN transceiver. The transceiver simulation model covers all required functions such as temperature monitoring, and bus failure detection. It has a complex structure with similar behavior as the physical model.



Figure 4: Block diagram of a CAN transceiver from Infineon Technologies AG

Common mode choke simulation model

Common mode choke coils placed between transceiver and the bus line help to filter out common mode signals noise produced by RF noise and non-perfect transceiver driver symmetry (NXP-Semiconductors 2006). In (Nguyen et al. 2008), the coupling factor between two wires in the choke is proved to have a very big impact on the signal integrity on CAN bus. Choke coil also becomes an important component at the CAN physical layer. The choke coil model was also developed with VHDL-AMS based on the spice model provided by EPCOS. Therefore it has a very accurate behavior.

Transmission line simulation model

One of the critical parts in the simulation test bench is the transmission line simulation model (Lorena Diaz 2005). The transmission line model is modeled with VHDL-AMS. The model parameters (e.g. characteristic impedance, propagation delay, length etc.) are characterized and determined via measurements. The star cable tree is then modeled by single transmission line model with different length connected together. This can be easily achieved by using SystemVision Schematics/Designes entry.

MODELLING OF THE CAN SYSTEM MEASUREMENT ENVIRONEMENT

In order to achieve a good match between measurement and simulation, not only the core components of the CAN physical layer are carefully modeled but also the measurement environment (e.g.: measurement probes, CAN triggering module termination resistor and CAN frame generator) of the 8-node CAN system is taken into consideration.

The measurement probes model

Probe basically provides a physical and electrical connection between measurement point/signal sources to an oscilloscope. A passive voltage probe has a typical equivalent circuit as shown in Figure 5



Figure 5: Equivalent circuit of a typical passive voltage probe

Measurement probe of oscilloscope is modeled by a capacitor connecting in parallel with a high-ohmic resistor. During the verification process, a comparison between active probe and passive probe is carried out, showing that better measurement results and better matching can be achieved when using active probe. Active probe has basically very low input capacitance and resistance with some compensated network compared to passive probe. In this paper, the two measurement probe models are different only in their capacitance and resistance values.



quantity v_pm across i_pm through p to m;

begin

i_pm==c*v_pm'dot; end;

Listing 1: An example of capacitor model by using VHDL-AMS modeling language

CAN triggering module termination resistor

For the measurement of the CAN network, a CAN triggering module from LeCroy is used besides the oscilloscope. The CAN triggering module is a CAN node that is set to filter and provide triggering signal when certain conditions are met. It interfaces with the CAN bus by a twisted pair with its own 1200hm termination resistor. For the verification of the 8-node CAN network in this paper, this termination resistor is considered as a part of the simulation system. Otherwise, it will show different in amplitude of the compared signals. This phenomenon has been observed and simulated at the beginning of our modeling process. The resistor is modeled exactly at the point which it is connected in the network.

CAN frame generator

The CAN transceiver input is CAN frame (CAN which generated from message) is CAN microcontroller. In Figure 6, it shows a CAN message recorded from the 8-node CAN network. It is important to keep in mind that, the CAN microcontroller is not simulated in this work. The transmission speed of a CAN network in reality is decided by the CAN microcontroller. One can measure the transmission speed by measuring the duration of a single bit on a CAN frame. For example, if a CAN bit has duration of 2 microseconds; the transmission speed is 500kbps.



Figure 6: Example of a CAN frame recorded from the 8-node CAN network

In order to model the CAN microcontroller output to an abstract level, it is necessary to be able to reproduce exactly at least the smallest bit in a CAN frame which is really generated by the CAN microcontroller. This is the whole idea of modeling the CAN frame generator whose generics are the bit duration (to determine the transmission speed) and the ramping time from 0 to 1 level. The CAN frame generator model generics were carefully configured as exact as the measurement value of a CAN frame bit from the real microcontroller. By this way, we can be certain that the microcontroller is not necessary to be simulated, hence it saves time and complexity for the simulation but still can produce a reasonable simulation results.

THE 8-NODE CAN NETWORK SIMULATION TEST BENCHES

Each of the models is created with a graphical symbol. This helps the simulation test benches in this work to be setup easily with Schematics/Designs entry of System Vision. All the simulation models described in the previous sections are connected together exactly the way they are arranged in the measurement setup as shown in Figure 7. A transient simulation is then performed. With the test bench, it is possible to setup different network topologies with a variety of cable stub length or different transmission rates and simulate them.



Figure 7: The 8-node CAN network simulation test benches with Schematics/Designs entry from System Visions of Mentor Graphics

Major differences between measurement and simulation setup are power supply, battery voltage sources and ground. In simulation test bench all of the electric sources and ground are set to be ideal.

VERIFICATION OF THE EIGHT-NODE CAN PHYSICAL LAYER STAR NETWORK

Verification of CANHi and CANLo signals at star connection point

In this section, comparison between measurement and simulation signals at the star connection point (CANHi and CANLo) is discussed. The results of measurement and simulation are compared by plotting in the same figure. The first verification is carried out on the 8 node CAN star network operated at 500Kbps transmission rate. The comparison shown in Figure 8 shows that deviation between measurement and simulation is quite small. However, when looking close to the behavior of the CANHi and CANLo signal changing from dominant to recessive mode, it shows a faster switching behavior by measurement than simulation. In order to fit the simulation curves, different values of the capacitors used in the measurement probe models were simulated. Decreasing the capacitance value results in a faster switching behavior of the CANHi and CANLo signals in simulation. A new measurement is then performed by an active probe and the same simulation test bench is simulated again with the new value of the capacitor (0.95pF) and resistor (1.0MOhm) from the active measurement probe.



Figure 8: A full CAN bit comparison of CANHi and CANLo signal at star connection point of 8 nodes CAN network (500Kbps transmission rate) using <u>passive</u> measurement probe (10.0 MOhm + 9.5pF)

In

Figure 9, it shows a new comparison between measurement and simulation when using an active measurement probe model.



Figure 9: A full CAN bit comparison of CANHi and CANLo signal at star connection point of 8 nodes CAN network (500Kbps transmission rate) using <u>active</u> measurement probe (1.0 MOhm + 0.95pF)

The matching of switching behavior from dominant to recessive mode of CANHi and CANLo signal is

significantly improved with the model from active measurement probe.

The same setup of measurement and simulation is applied for verification at transmission rate of 1.0Mbps. Once again, it shows a very good matching between measurement and simulation results of CANHi and CANLo signals at star connection point in Figure 10.



Figure 10: A full CAN bit comparison of CANHi and CANLo signal at star connection point of 8 nodes CAN network (1.0Mbps transmission rate) using active measurement probe (1.0 MOhm + 0.95pF)

Simulation of Tx and Rx signals of the CAN micro controller interface

The CAN system used in this paper can visualize the whole CAN protocol up to application layer. As mentioned above, this CAN system is mainly developed for the measurement purpose. The control pin RM is connected to 5.0V while the pin INH is connected to ground for a low level signal. By this setup, the CAN nodes are tested at their normal operation mode as shown in Figure 11.





As demonstration, a simulation scenario from Stand-by mode switching to Normal mode is performed. The control signal RM and INH are modeled by a piecewise linear voltage source (V_PWL). The RM signal starts

at 0.0 second and remains its 0.0 volt for duration of 2.0 nanoseconds and then it is switched to 5.0V for the rest of the simulation time (300 microseconds). In a similar way, the INH signal starts at 0.0 second with 0.0V until the 2^{nd} nanosecond, then it switches to 5.0V until 50.0 microseconds then it switches back to 0.0V for the rest of simulation time.



Figure 12: Simulation scenario of 8 node Star CAN network from Stand-by operating mode switching to Normal operating mode

With this setup as shown in Figure 12 (the 1st and 2nd windows correspond to RM and INH signals respectively), the simulation shows that the first 50 microseconds of the simulation time all the CAN transceiver are at the Stand-by mode because RM = high and INH = high. During this first 50 microsecond, bus voltage is 0.0V (please refer to Figure 12, the 3rd window which shows CANHi and CANLo voltage level) demonstrate that there is no communication between the 8 nodes regardless CAN bits from Tx pin interface of the CAN micro controller on NodeB are already transmitted (please refer to Figure 12, the 4th window which shows CAN bits transmitted from NodeB).





The 5th and 6th represents for the CAN bits received from NodeB and NodeD respectively. It shows also that the first 50 microseconds, NodeB and NodeD could not receive any CAN bits due to the CAN transceivers are set to Stand-by mode. For the last 250 microseconds of the simulation, all the CAN transceiver is set to operate at Normal mode because of the control signal state RM=high and INH=low (please refer to Figure 11).

By comparing CAN bits transmitted and received in the 3^{rd} , 4^{th} , 5^{th} windows of Figure 13, it shows that all the bit transmitted from NodeB are received by NodeD and NodeB itself (CAN is a serial broadcast communication protocol). All the received CAN bits at NodeA to Node H are checked however they are not shown here due to writing space limitation. Electrical signal CANHi and CANLo of CAN bus at star connection point are also correctly demonstrated based as described in Figure 1, excepted some the first several CAN bits which are not 100% matching to the nominal voltage level on CAN bus. This is explained by the electrical transient switching behavior of the CAN transceiver.

CONCLUSION

With the implementation the new choke coil BS82789C513 with a very high value of the coupling factor and a proper termination circuit, the star configuration topology described above shows a quite stable behavior of the electrical signal on the CAN physical layer. The good matching between measurement and simulation once again proves that the models used in the simulation system are accurate and very reliable. Models of measurement probe, the CAN triggering module termination resistor as well as the CAN frame generator model should not be ignored when performing the system modeling, simulation and verification against real measurement.

The described modeling methodology also shows that the CAN physical layer is able to be simulated up to the interface of the CAN microcontroller without having to model and simulate the CAN controller. This is a real advantage in reducing the complexity of the simulation system, thus reducing the computational effort and simulating time.

The next part of this work will focus on using these accurate simulation models to investigate the behaviors of a larger CAN network with different types of topology (linear bus, star or hybrid) at different transmission speed. Bus error detection and network delay analysis by using simulation will be also the next steps.

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CALCULATION OF ALERT LEVELS FOR RELIABILITY

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KEYWORDS

Aviation, Reliability

ABSTRACT

Safety in Aviation is a forecast of failure. That's why many situations occuring during the whole exploatation are noticed and analysed. Analyse is devided in to many factors and, as every statistic use as many data as possible. To get any conclusions one have to compare results of analyses with established alert levels. Those alert levels are a picture of wider experience. The paper describes how to make such a picture. After one simulates when some component will failed, one can replace the component by new one before failure.

INTRODUCTION

Reliability engineering and maintenance are the source of safety. They are one of the most important aims in modern aviation. The modern reliability engineering is also the way of seeing safety as exploitation costs reduction. Following good written reliability programs airplanes earning money as long as possible, as often as possible. They are not spending time waiting for parts, which were unexpectedly broken, they are reaching destinations on time. The customers are glad because of accuracy and reliability. How to reach this aim?

PROBLEM FORMULATION

Safety in Aviation is a forecast of failure. That's why many situations occuring during the whole exploatation are noticed and analysed. Analyse is devided in to many factors and, as every statistic use as many data as possible. As many data as possible it means that operators shuold share to each other with thay problems, failers, mistakes and all ashamed accidents which can be usefull for reliability statistics. That's why all participants have to make some Proprietary Information Agreement to protect Shared Data from Misuse. Misuse it means for instance marketing, competitors activity analysys and so on.

To get any conclusions one have to compare results of analyses with established alert levels. Those alert levels are a picture of wider experience, experience of a big amound of same type aircrafts.

The Reliability Report is required by aviation authorities from every operator. For European countries authority is the EASA (European Aviation Safety Agency) and for USA it is the FAA (Federal Aviation Agency). Reports in most cases reach authorities every month, for every aircraft, from every operator. Reports differ between each other depending on type of aircraft, number of aircrafts operated in company, number of hours flown, tape of missions and so on. What form and kind of data will appear in report is written in Reliability Programs accepted by aviation authorities and created by operators, but in every report there are such data as hours flown by each aircraft, number of landings, number of defects and accidents, schedule interruptions, delays, cancellations, air turnbacks, and diversions and reporting

GROUPING AIRCRAFT SYSTEMS

All of reported defects have to be divided using ATA code. The Ata code is the System (two digids), subsystem (four digids) or Component (8 digids) Code Table DEVELOPED by The Air Transport Association of America (ATA), and called Specification 100 code. Now it is used By FAA and accepted by EASA. Such

fragmentation is useful when you want to know what part of the airplane, what system or what component most common makes problems, where you have to look more often. The main system is as follows:

21 Air conditioning

22 Auto Flight23 Communications

24 Electrical Power

25 Equipment Furnishing

- 26 Fire Protection
- 27 Flight Controls

28 Fuel

29 Hydraulic Power

30 Ice & Rain

31 Indicating & Record

32 Landing Gear

33 Lights

34 Navigation

- 35 Oxygen
- 36 Pneumatic

37 Vacuum

- 38 Water / Waste
- 45 Central Maintenance
- 49 Auxiliary Power

51 Structures

- 52 Doors
- 53 Fuselage
- 54 Nacelles / Pylons

55 Stabilizers

56 Windows

57 Wings

- 71 Power plant
- 73 Engine Fuel Control

74 Ignition

76 Engine Controls

78 Exhaust

79 Oil

80 Starting

As it can be seen there are only some chosen chapters, and in every chapter there are also subchapters. The system is independent on aircraft type so if some operator frequently have to change parts in its different type of aircraft's, so with different Part Numbers it is simple to check if, for instance there is permanent problem with landing gear system. Then one can ask if it is a maintenance problem or exploitation or conditions problem. But this question is to answer using system other then ATA 100. A mean for all aircrafts, operators and conditions on all over the world is, that on the first place are:

- 1. ATA 32 Landing Gear;
- 2. ATA 34 Navigation;
- 3. ATA 24 Electrical Power;
- 4. ATA 27 Flight Controls.

It does not mean that those are the main reasons of crashes, but dalays, flight cancelations or just aims for line maintenance.

RALIABILITY FACTORS

The reliability factors can be divided in 3 groups. The first group contains factors describing whole aircraft and people who are somehow connected with the aircraft, pilots, management, and maintenance. In this group one can find such factors as:

- PRR (Pilot's Reports Rate) Factor

This factor shows how many defects or problems were reported/found by pilots. Some of defects appeared during the flight but there is also group of cases, where the problems were found by pilots because they were not found by mechanics. The parameter is given as cases for 1000 flights.

- PRMR (Pilot's Reports/Maintenance Report) Factor

This factor show how many defects or problems were reported/found by pilots in compare to defects found by maintenance departments.

- DR (Dispatch Reliability) Factor

This factor analyses technical reason influence on dispatch delays/cancelations compare to all delays/cancelations.

- SR (Shop Rate) Factor

Factor shows amount of time when aircraft spend on unplanned maintenance every 100 flight hours.

- TF (Technical Functionality) Factor

The TF Factor is number of hours flown with accepted defects and flight limitations (Flight with Minimum Equipment List Regulation, and Hold Item List Document usage) for every 100 flight hours.

- TI (Technical Incidents) Factor

This factor is calculated for 1000 flights. The deference is because of calculated case. It is a serious defect with influence on flight safety, which should be report in separate report to authorities.

The second group contains factors, which more precisely describe aircraft and its components. Every of factor below is calculated separately for each ATA 100 chapter or, in case of number of defects/removals/shop time even subchapters. In this group one can find following factors:

- RR (Removals Rate) Factor

The RR factor show number of removals of exact component from an aircraft, independently of reason for this removal for every 1000 cycles or working hours.

- FR (Failure Rate) Factor

The FR factor shows number of removals of exact component from an aircraft, because of failure for every 1000 cycles or working hours

- MTBR (Mean Time Between Removals) Factor

The MTBR factor, as the name says show average time between removals of exact component from an aircraft for every 1000 cycles or working hours.

- MTBF (Mean Time Between Failure) Factor

The MTBR factor, as the name says show average time between removals of exact component from an aircraft, because of failure for every 1000 cycles or working hours

- <u>MTBUR (Mean Time Between Unscheduled</u> <u>Removals) Factor</u>

The MTBR factor, as the name says show average time between unplanned removals of exact component from an aircraft for every 1000 cycles or working hours.

The third group of factors is the group of factors combined with power plants. Those very important aircrafts components have separate factors.

- IFSD (In-Flight Shut Down Rate) Factor

Factor describing number of In flight shut down of engines or other serious problems with engines during flight. Because the case is not very common the factor is calculated for 1000 flight hours.

- URR (Unscheduled Removals Rate) Factor

This factor is unscheduled engines removals from an aircraft rate. The factor differs from previous one, because removal can be made also after defect find on ground. The factor is calculated for 1000 flight hours.

- SVR (Shop Visit Rate) Factor

This is a parameter showing number of engine repairs in a shop for 1000 flight hours.

AGE RELIABILITY PATTERNS

Analyzing changes of the parameters during life of components one can found that some components aging in different way than others. This is only sometimes obvious, usually which component is accurate to which curve one knows after looking in to statistics. The typical curves can be divided in two groups. In first group one can find components with limited age, or, where setting age limit is reasonable, the second, much more common, where not. The first group examples are:

1. The Bathtube Curve:



Infant mortality, followed first by a constants or gradually increasing failure probability and then by a pronounced "Wear Out" region.

An age limit may be desirable, provided a large number of units survive to the age at which out begins. Such curve is respond to 4 % of components only.

2. Constant or gradually increasing failure probability, followed by a pronounced wear out region. Such curve is respond to 2 % of components only.



 Gradually increasing failure probability. No change in characteristic in age, but setting limit is reasonable. Such curve is respond to 5 % of components only.



Those 3 types are together 11% of all components, and only this amound require setting time limits in maintenance programs.

Secound group are the cases where setting such limit is not reasonable:

1. Low failure probability when the item is new or just out of the shop, followed by a quick increase to a constant level.



Such curve is respond to 7 % of components only.

2. Flate rate. Constant failure probability during years/ flight hours/ cycles.



Such curve is respond to 14 % of components.

3. Infant mortality, followed by a constant or very slow increasing failure probability. This is valid for 68% of all components and is typical to electronic equipment.



The second group is 89% of all cases.

ALERT LEVELS CALCULATIONS

There are several methods of calculation alert levels, all of them are well known as statistical error calculation. Main or most common are:

- 1. MEAN + 3 SD
- 2. MEAN + STANDARD DEVIATION OF MEAN OF MEANS + 3 SD
- 3. MEAN x 1,3
- 4. MEAN + 2 SD
- 5. Weibull Method

As the errors are used for foresight they have to be racalculeted after getting new data. It depending on operator how often alert levels have to be recalculated. Most common case is every month, but some companies recalculated alert levels every three months or even every half a year, depending of flight hours does the fleet fly every month.

CONCLUSIONS

Lot of the presented factors is similar and the choice which is more useful for an operator or airlines depends on operator its self and authorities which have to accept the Reliability Program. Factors can also be created especially for operators needs or problems they think are more common. But the most important thing is to analyze the changes of calculated factors during time, after each probe and compare it to reliability levels predicted by previous years of flying on analyzed aircraft and results for rest aircraft the same type which are flying all over the world, whole manufactured fleet. The simulation is as proper as large is the number of cases the statistics data used for this simulation is based on.

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AUTOMATIC TRAFFIC DETECTION SYSTEM

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KEYWORDS

Traffic detection, image processing, traffic modelling, image analysis

ABSTRACT

This article presents the concept of automatic traffic detection system. Idea of the system is based on image processing and distributed database. This work focuses on presentation of test installation set-up.

INTRODUCTION

Nowadays, systems for automatic identification and vehicle control are used around the world. There are used various measuring techniques, such as loops or radars. Most of them need a special infrastructure to operate. Therefore, the systems based on image processing are used more and more frequently.

Image processing based systems can be used for:

- automatic counting, detection and classification of the vehicles,
- traffic management assistance,
- control systems and toll collection.

An essential element of those system is an ANPR (Automatic number plate recognition) module. This module uses the image from the camera to automatically read the registration number. While using this technology, fast and reliable identification of the vehicle is possible.

SPECS is an example of the solution mentioned above. This system was created in Great Britain in 1999. The system is able to detect vehicles in subsequent segments of the road using a network of cameras. The system allows detecting vehicles in subsequent segments of the road using a network of cameras. Consequently, it can estimate average speed of the vehicle using information from number plate registration module. Moreover, it enables detection of speed limit violations.

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The results of their operation in different areas of Great Britain showed significant improvement in security. On the roads under control, the number of static accidents fell by more than a half. Compliance with the recommended speed for drivers additionally improved traffic flows.

Another example of a similar system is the system Safe-T-Cam that belongs to the Roads and Traffic Authority in Australia. It was established in 1995 with the purpose of limiting the number of accidents involving heavy vehicles by detecting such offences as:

- violations of speed limits
- driving outside the designated hours of driving
- detecting unregistered vehicles

The system consists of twenty four cameras installed on the main roads of New South Wales.

In addition to these, there are also analogous systems in other countries, including Trajectcontrole (Netherlands), Tutor (Italy), Abschnittskontrolle (Austria).

CONCEPT OF THE SYSTEM

The basic elements of the system are a camera and a small computer. This device realizes several crucial functions for the system. Firstly, it is used as a capturing device which grabs visual data from the camera. Secondly, it is used as a processing unit, which runs an image processing algorithm. As a result, it returns information data about vehicle: direction of the move of the car, the time of appearance of the car and type of it. Subsequently, the calculated results are stored into local database and each two minutes are sent by GSM to data warehouse on the server. Then, based on these data, system draws diagrams and displays them on website. These diagrams can be used to analyse monthly, weekly or daily density of the traffic.

TEST INSTALLATION

The main goal of the installation was to provide information about the traffic on the main road leading through the city. The primary objective was to provide
information on vehicles entering or leaving the city. This would enable the tracking of both local and transit traffic for local authorities.

Originally the device was supposed to be installed in the following locations (Figure 1).



Figure 1: Planned device locations

Unfortunately, the implementation of the assembly resulted in a number of problems. First problem was the inability to mount devices on street lighting poles.

Another considered variant was to build some dedicated poles for devices along the road. Unfortunately, such an option was also abandoned due to problems with the permission from the provincial roads management office.

Some alternatives were considered for the power supply. The first option was to connect device to a power source of lighting poles. The specification of this connection is that the power supply of the lighting poles is only available in certain parts of a day, because the lighting is integrated with a global switch that turns the power on or off across the lighting network. While the change in the rules governing the activities of this network does not make sense, it seems reasonable to use this lighting to power the device. It is possible to use gel batteries, the load during operation of the lightning and power supply unit when there is a lack of power.

An additional positive aspect is the characteristics of the power consumption of the device. The main element that consumes electricity in the device is heating. This element requires the vastest amounts of power in winter and at night, during a period where it can be powered directly from electricity network. For instance, in summer, when the device operating at power from the battery is the longest, it is also when device have the lowest power consumption (comparing to other seasons). It is also possible to use the power installation using batteries and solar batteries.



Figure 2: Final device locations

In view of these problems the device was assembled on existing city office infrastructure. For this purpose we used the city office buildings and connected devices to the existing electricity network of those buildings. The final locations of devices are illustrated on figure.

In fact, the space for mounting the devices is not optimally selected from the point of view of maximizing the effectiveness of the system. They were selected from strictly limited possible sites of operation.

After launching the devices, it appeared that problems connected with lighting and coping with weather conditions occurred. The first device was mounted in a way that is directly positioned at a short piece of road.



Figure 3: Image captured by first device.

It was a true test for the algorithm but there were no problems with the reduction of visibility (rainfall, glare of the sun, street light).



Figure 4: Night



Figure 6: Fog

In contrast, in the case of the second device has a problem with both rainfall and with the glare. It resulted from the position of the main camera, which is set to observe a larger area of the road.

ANALYSIS OF COLLECTED TRAFFIC DATA

Information about traffic are collected in data warehouse. Based on these data, system draws diagrams and displays them on the website. These diagrams can be used to analyse monthly, weekly or daily density of traffic. Figure 8 shows weekly density of traffic in Jabłonowo Pomorskie. Data is collected on 26.02.2009 at 15.19.

Nowadays the rules, which regulate measurement of traffic concentration are based on temporal (in our opinion not sufficient enough) measurement in specific hours and days. Then the results are used to enumerate average number of cars of all categories, such as cars, lorries, buses or tractor-trailers, during whole day. There are some constant factors, which help to make this calculation as reliable as possible. Even though, the



Figure 5: Sunlight



Figure 7: Rain

results could be more accurate if this measurement would be carried during the whole day or week.

Our solution gathers information about traffic type and intensity, which can be used to make needed statistics. Besides, our device offers more functionality. For instance, it can be placed in the main crossroads of the city and thanks to it, model traffic in the city.



Figure 8: shows weekly density of traffic in Jabłonowo Pomorskie.

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TOWARDS THE AUTOMATED INFERENCE OF QUEUEING NETWORK MODELS FROM HIGH-PRECISION LOCATION TRACKING DATA

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KEYWORDS

Location Tracking, Spatiotemporal Data Sets, UWB, RFID, Data Mining, Workflow Induction, Queueing Networks, Performance Modelling

ABSTRACT

Traditional methods for deriving performance models of customer flow in real-life systems are manual, timeconsuming and prone to human error. This paper proposes an automated four-stage data processing pipeline which takes as input raw high-precision location tracking data and which outputs a queueing network model of customer flow. The pipeline estimates both the structure of the network and the underlying interarrival and service time distributions of its component service centres. We evaluate our method's effectiveness and accuracy in four experimental case studies.

INTRODUCTION

Stochastic models, especially queueing networks, have been widely used to model and analyse the performance and reliability of systems that involve the flow and processing of customers via a network of service centres. Indeed such models provide a powerful "virtual laboratory" for identifying and explaining bottlenecks in existing systems and for exploring the impact on performance of proposed changes to those systems, e.g. changes in customer flows, the number and allocation of resources, system workload, scheduling policies and so on.

Traditionally, constructing a performance model is a four step process: conceptualisation, parameterisation, validation and analysis. The first two steps are essential in building an accurate model, which in turn is crucial in giving confidence in the output of subsequent steps. However, they are typically time-consuming, expensive, intrusive, labour-intensive, and prone to bias and other errors. The limited amount and low quality of manuallycollected data often lead to an inaccurate picture of resource flows and poor estimations of model parameters.

In recent years, wireless location tracking technologies based on RFID (Radio Frequency Identification) and UWB (Ultrawide-band) have been increasingly deployed to collect real-time location tracking data. For example, RFID has been applied in patient identification (Chen et al., 2005) to enhance the efficiency and effectiveness of management in hospital Emergency Departments. Combined technologies, such as sensor networks and RFID, have also been deployed, for example in a hospital blood bag management system that continuously monitors the temperature of stored blood bags as well as their locations (Kim et al., 2006). These technologies offer the advantage of collecting large amounts of high-quality location data in an inexpensive and non-intrusive way. This data is a valuable input in building performance models that can better characterise the operation of real systems.

Raw location tracking data usually contains noise and other extraneous information; thus appropriate data processing methods are necessary for extracting useful information from it. Much research work (such as Gonzalez et al. (2006a), Gonzalez et al. (2006b) and Gonzalez et al. (2006c)) has been done in designing new data models to facilitate RFID data warehousing and inferring highlevel information from RFID data, such as probabilistic item flows. However, RFID data has some distinct characteristics when compared to the location tracking data collected by other location tracking technologies, such as sensor networks. In the former case, the location reads of an RFID-tagged item have strict spatial relationships with the RFID readers, as a tagged item's location can only be known when it is scanned by an RFID reader, the location of which is usually fixed. By contrast, in the latter case, the location data is a noisy and frequently incomplete trace of the tagged entities' geographical locations; spatial relationships and interactions between tagged entities must be inferred on the basis of proximity or otherwise.

The aim of our work is to automatically extract a queueing network model of customer flow from observations of a real-life system gathered using a high-precision location tracking system. To achieve this, we present an approach based around a four-stage data processing pipeline, whose initial input is raw location tracking data, i.e. a spatiotemporal data set giving the observed location of tags at various times. The first two stages of the data processing pipeline remove irrelevant location information and use tagged entities' geographical locations to infer high-level spatiotemporal relationships among customer and server entities (including the presence of customers in the service area of servers and customer movements between servers). The third stage of the pipeline extracts occurrence times of arrivals and departures of

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) customers at servers. The fourth stage uses these times to estimate the underlying interarrival and service time distributions of the original physical system, and also infers routing probabilities from customer movements. Together, these yield a parameterised queueing network model of the real-life system.

For the purpose of evaluation, we conduct four case studies corresponding to simple queueing systems with known structure and parameters. Goodness of fit tests are used to assess whether the extracted distributions of interarrival time and service time exhibit the same probabilistic characteristics as the real ones.

The remainder of this paper is organised as follows. The next section introduces previous research literature closely related to our work. This is followed by a brief description and comparison of three common location tracking technologies – RFID, WiFi and UWB, of which UWB is our adopted technology. We then describe and illustrate each stage of the developed data processing pipeline, discussing issues encountered during implementation, before presenting four case studies. We conclude with a summary of our results and a discussion of potential future work.

PREVIOUS WORK

Our work shares some high-level similarities with previous research efforts on mining RFID data. These research efforts have been focused on efficiently extracting flow information from massive RFID data sets through innovation of data model design and data compression techniques. For example, Gonzalez et al. (2006c) proposed a new data model for data-warehousing RFID data sets. Their goal was to enable the efficient storage and high-level querying of such data sets, taking into account the fact that several items may be aggregated into single tagged units. Building on this work, Gonzalez et al. (2006a) further presented a method to build up a warehouse of item flows, which is referred to as flowcubes. The flowcube is different from traditional data cubes in that its measure is not a scalar aggregate but a flowgraph, which is a tree-shaped graph that maintains the path information of the item flow. Each node in a flowgraph represents a location and edges between nodes correspond to transitions between locations. Gonzalez et al. (2006b) later presented a method to construct compressed probabilistic workflows that describe the general movement paths of items, as well as the significant exceptions. Although our data bears different characteristics from RFID data, our approach is also directed at devising a method to extract flow information from location tracking data.

Workflow induction and process discovery are also closely related research areas. These areas explore techniques that can use event data, which records the activities of an on-going process, to build up a formal model that describes the process's behaviour. Cook and Wolf (1995, 1996) proposed three methods, ranging from the purely algorithmic to the purely statistical, to discover and produce formal models corresponding to actual process executions. In contrast to the finite state machine approach of Cook and Wolf, Agrawal et al. (1998) presented an algorithm that uses existing execution logs to model the workflow structure of a given business process as a graph.

Other research work has been conducted in inferring performance models from sample executions. Instead of using pure statistical learning methods, Zhang and Bivens (2007) and Zhang et al. (2007) incorporate domain knowledge into machine learning techniques such as Bayesian networks and neural networks for response time modelling. Sen et al. (2004) present a machine-learning algorithm that can learn the underlying edge-labelled continuous-time Markov chains of a stochastic system based on sample execution trace data.

Our work seeks to develop a data processing method that incorporates the strengths of statistical learning techniques with the aim of extracting service and interarrival time distributions and routing probabilities from location tracking data; together these will specify a queueing network model of customer flow with enhanced accuracy.

LOCATION TRACKING TECHNOLOGIES

Three common technologies that have been employed in location tracking are RFID, UWB and WiFi. The various technologies used in real-time tracking have distinct characteristics which lend them to differing applications. RFID is usually passive, which means that a RFID tag has to be scanned by a reader for its location to be recorded. Tracking with WiFi typically provides an accuracy of the order of 2–7m in 2D while the latest UWB-based systems provide greater accuracy of around 15cm in 3D; the latter allows for detailed detection of customer/server interactions and gives potential to model processes such as contact-based spread of pathogens. WiFi-based systems are, however, often easier to deploy as they use hardware (WiFi access points) that might already be installed.

UWB operates over the frequency range 3–10 GHz in the U.S and 6–8.5 GHz in Europe (The Federal Communications Commission, 2002). Interference with other signals is prevented as UWB emits short-duration highbandwidth radio pulses at a low power making it particularly suitable for use in radio sensitive environments such as hospitals. The low power does, however, limit the range over which detection is possible but is still able to penetrate walls. The short length of time over which a pulse is emitted also means that a high density of devices can be achieved in a given detection area. Calculation of the location of a tag is performed using time difference of arrival (TDOA) and angle of arrival (AOA) of the radio frequency pulses at different sensors (Ubisense) (cf. Figure 1).



Figure 1: UWB-based sensors and tags (left) use a combination of angle-of-arrival and timed-difference-of-arrival triangulation schemes to enable high-accuracy tag location tracking (right)

INFERRING PERFORMANCE MODELS FROM HIGH-PRECISION LOCATION TRACKING DATA

Data Processing Pipeline

This paper presents an automated four-stage data processing pipeline. The input to our pipeline is the raw location data from a real-life physical system (gathered via a high-precision UWB-based sensor network) and the output is a queueing network describing customer flow in that system. This queueing network is specified by routing probabilities and interarrival and service time distributions estimated from the location data.

Figure 2 gives an overview of the data processing pipeline. The input and output data of each stage are stored as database tables, which are designed to facilitate data querying and further manipulation. After each stage is completed, the inputs from the previous stage can be discarded.

Stage 1

Raw location tracking data is stored in the **Traces** table as a stream of tuples of the form (tagName, type, time, x, y, z, stderr).tagName is a unique identifier for each tag and type refers to the category a tag belongs to. In this research there are two types of tagged entities of interest: Server and Customer. Server entities are those offering services or resources in a system; Customer entities are those requesting services or resources. time is the timestamp when the location update took place; ideally this is a taken using a high-resolution timer with millisecond resolution or better. x, y, z are the locations of the tags expressed in a Cartesian coordinate system. stderr expresses the location tracking system's estimate of how much the measured location might deviate from the actual location.

Using the type field in the table, the **Traces** table can be split into the **Server Traces** table and the **Customer Traces** table, which store the location tracking data for Server and Customer entities, respectively. The data stored in both tables is of the form (tagName, time, x, y, z, stderr) and is sorted by time. Furthermore, in Stage 1, linear data interpolation is conducted to fill out gaps in trace data when two contiguous location updates for a tag take more than four times longer than would be expected (in our case tags should update their position four times a second).

Stage 2

After the first stage of the data processing, the data is still very low-level. The main purpose of the second stage is to extract relevant higher-level data. This includes at what time a customer arrives at a server, when the server finishes serving the customer and the number of customers being served or queueing for service at a server at a specific timestamp. We assume each server in the system has a user-defined service area, which is a circular area with given radius. If a tag is detected within the service area of a particular server at a given timestamp, we assume that the customer entity that owns the tag is either being served by the server or is waiting to be served in the queue of the server. If the tag is found to be located within user-specified entry or exit areas, the customer entity corresponding to the tag is considered as entering or leaving the system. In other cases, the customer entity is assumed to be moving between servers and/or entry/exit areas.

The outputs of the second stage of data processing are **Service Load Traces** tables (one table for each server) and one **Customer Location Traces** table. The contents of these two types of table are as follows:

Service Load Traces tables The data stored in these tables is of the form (time, count, (customer list)) and is ordered by time. The count field is the total number of the customer entities that are located inside the server's service area at the given timestamp. The field (customer list) maintains the tag IDs of the customer entities. Table 1 gives an example of the Service Load Traces table.

The main challenge in this stage of data processing is that location tracking data in reality does not appear as a smooth trace describing the object's path;



Figure 2: Four-stage data processing pipeline

time	count	customerlist
13.3163	1	Customer0
13.4882	1	Customer0
13.6633	0	
13.8360	1	Customer1
13.9894	2	Customer1,Customer0
14.1501	2	Customer1,Customer0
14.3084	2	Customer1,Customer0
14.4703	2	Customer1,Customer0
14.6341	2	Customer1,Customer0

Table 1: Example Service Load Traces table

noise and other artefacts such as radio reflections might result in location updates with sudden deviation from the actual locations. The erratic location updates might lead to the conclusion that a customer entity has entered the service area when in fact it has not. A window-based voting mechanism is therefore used to avoid this situation. In each time window, defined as the time between two Server location updates, there is one counter for each entity that has visited the service area of a certain Server. Assume that there are more than one location reads of a customer tag, say Customer 1, between two timestamps t1 and t2. When checking whether Customer1 was inside the service area of a Server, say Server1, its counter value is incremented by one if Customer1 is detected inside Server1's service area and decreased by one if not. If at time t2 the value of the counter is positive, it means that there are more readings between t1 and t2 supporting the notion that Customer1 is within Server1's service area. If the counter's value is negative, then Customer1 is not included in (customer list).

Customer Location Traces table The data stored in this table is of the form (tagName, time, location) ordered by time. Instead of exact Cartesian coordinates, the location information is reduced into a higher-level description. For example, as shown in Table 2, we can see that Customer1 is moving at time 13.2983 and Customer0 is within a service area of Server3 at time 13.4027.

tagName	time	location
Customer1	13.2983	moving
Customer2	13.3847	moving
Customer0	13.4027	Server3
Customer1	13.4194	moving
Customer2	13.4405	moving
Customer0	13.4631	Server3
Customer1	13.5592	moving
Customer2	13.5816	moving
Customer0	13.6023	Server3
Customer1	13.6240	moving

Table 2: Example Customer Location Traces table

Stage 3

The major work in this stage is to detect arrival and departure events from the **Service Load Traces** tables and calculate customer interarrival times and service times. We process each record in each **Service Load Traces** table and detect any differences in the $\langle customer list \rangle$ fields between two contiguous records. For example, if at timestamp t1, the $\langle customer list \rangle$ field is $\langle Customer0, Customer1, Customer2 \rangle$ and at the next timestamp t2, the $\langle customer list \rangle$ field is $\langle Customer1, Customer3 \rangle$, then between t1 and t2 there might be one arrival event of Customer3 entering the service area and two departure events of Customer0 and Customer2 leaving the service area.

However, a missing tag ID in the (customer list) field does not necessarily represent "real" departure events. Infrequent location updates or erratic location reads of the tags between two contiguous timestamps might contribute to this phenomenon. In this case, the missing tag IDs should still remain in the (customer | list \rangle field. In order to judge whether a real departure event occurred, a look-ahead action is taken; this is essentially a query to the Customer Location Traces table to check whether the missing Customer entity shows up again in the server's service area within a certain amount of time from the current timestamp. The amount of time is based on the minimum time for a customer entity to make a round trip from the current server to the entry/exit areas and back to the current server, and is another usersupplied input.

For arriving customers, it is assumed that database entries represent true arrival events. This is because of the window-based voting mechanism applied in the second stage of data processing.

The next step after detecting a customer arrival or de-

parture event is to estimate the most probable time when the event occurred. The estimation of departure event occurrence time is the average of two values, both of which are obtained from querying the Customer Location Traces table. The first value is called first disappearance time. It refers to the first timestamp at which the customer's location is not inside the server's service area after it begins service. The second value is called the last appearance time, which is the last timestamp at which the departing customer remained in the service area between its service start time and the first disappearance time. A similar approach is used to estimate arrival times using the last time the customer was observed outside a service area and its first appearance time within the service area. We note the differences between the two times were typically not as significant for arrivals as for departures, since the tags we use are designed to update their positions more frequently whilst moving.

The outputs of the third stage are the extracted interarrival time and service time samples for each Server.

Stage 4

The data stored in the Customer Location Traces table can be seen as a stream of event logs that trace all the activities of the Customer entities in time order. Stage 4 uses this table to mine the structure of customer flow in the system by a method that is a simplified adaptation of the workflow mining methods proposed by Agrawal et al. (1998). One feature worth noticing is that tags can be "recycled" after the tracked customers leave the system, so one tag ID can actually represent different customers. It is therefore necessary to identify the entry and exit points of customer flow in the system. The mining process is basically a counting process. As each record in the Customer Location Traces table is processed, a tracking table is used for recording all the possible paths or sub-paths the customers have passed through so far, and the number of customers that followed a specific path. Table 3 gives an example of such a table. From it we can conclude that in this specific system, 27 out of 28 customers first visited Server1 while one customer first visited Server2. Among the 27 customers, 19 customers went on to Server2 next, while 8 proceeded to Server3. It is straightforward to estimate routing probabilities from such a table.

path	count	nextFlow
Server1	27	Server1
		Server2,
		Server1
		Server3
Server2	1	
Server1 Server2	19	
Server1 Server3	8	

Table 3: Example **Customer Flow** table

Having now identified the structure of a high-level queueing network through routing probabilities, the next step is to characterise the arrival process and service process associated with each (single-server) queueing node. We do this by fitting candidate distributions to the interarrival and service time samples generated in the previous stage of the pipeline. Specifically, we use the samples' coefficient of variation, c_v , as a simple indicator of the underlying distribution as follows:

- If c_v ≃ 0, the underlying distribution is likely to be deterministic.
- If $0 < c_v < 1$, the underlying distribution is likely to be hypo-exponential.
- If $c_v \simeq 1$, the underlying distribution is likely to be exponential.
- If $c_v >> 1$, the underlying distribution is likely to be hyper-exponential.

Having thus selected a candidate distribution, we use maximum-likelihood estimation to obtain distribution parameters. We then conduct three different goodness of fit tests, including Kolmogorov-Smirnov, Anderson-Darling, and Chi-squared tests, to measure the compatibility of the sample with the experiment's true probability distribution function.

CASE STUDIES

In this section, we perform evaluation and analysis of our data processing pipeline using four case studies. For each case study, we designed an environment whose customer flow resembles the one in a simple queueing system with known parameters. We then staged experiments where volunteers transported tags between single-server service areas at times sampled from known distributions. Positions of tags were continuously recorded using a Ubisense Location Tracking System. Figure 3 illustrates the structure and parameter settings of the approximated queueing systems.

We use the first three case studies to show that extracted interarrival and service time distributions are similar in statistical behaviour to the actual underlying distributions. We use the fourth case study to show how the proposed data processing method copes when inferring customer routing probabilities.

Results and Discussion

Figure 4 shows the historical paths of all tags during the first of our experiments. The tags' locations are colourcoded; the red positions indicate when the tag was moving, while the blue locations are when it remained (almost) static. From this, we can infer the locations of the service and entry/exit areas and the paths between them.

Service Time Distributions

Table 4 lists the coefficients of variation calculated from the extracted service time samples in the first three case studies, which are compared with the coefficients of variations of the actual underlying distributions.



Figure 3: The settings of the four case studies



Figure 4: Visualisation of the raw location tracking data from Case Study 1 to show moving tag positions (red dots) and static tag positions (blue dots).



Figure 5: Cumulative histograms of the extracted service time samples in the three case studies.

	Case Study 2		0	Case Study 3	
	Kolmogorov-Smirnov		Kolmogorov-Smirnov		
test statistic	0	.0855		0.0851	
α	0.1	0.05	0.1	0.05	
critical values	0.1526	0.1696	0.13	0.1444	
rejected?	No	No	No	No	
	Anders	son-Darling	And	derson-Darling	
test statistic	0.4121			0.4868	
α	0.1	0.05	0.1	0.05	
critical values	1.929	2.502	1.929	2.502	
rejected?	No	No	No	No	
	Chi-squared		Chi-squared		
test statistic	4	4.671	5.325		
α	0.1	0.05	0.1	0.05	
critical values	9.236	11.07	10.64	12.59	
rejected?	No	No	No	No	
estimated λ	0.0256 cust/sec		0.	0213 cust/sec	
actual λ	0.02833 cust/sec		hyper-exponential with		
			$\lambda_1 = 0.03333 \text{ (prob}_1 = 0.9)$		
			$\lambda_2 = 0.0$	0667 (prob ₂ =0.1)	

Table 5: The results of three goodness of fit tests at significance levels 0.1 and 0.05 applied to the extracted service time samples from Case Study 2 and Case Study 3. The null hypothesis is that the sample is extracted from an exponential distribution. The estimated λ is the rate of the best-fit exponential distribution (in cust/sec).

Case Study	c_v (estimated)	c_v (actual)
Case Study 1	0.17	0.00
Case Study 2	0.93	1.00
Case Study 3	1.15	1.57

Table 4: The coefficients of variation c_v of the extracted service time samples compared to their actual values

The designed probability distribution of the service time for Case Study 1 is deterministic. The calculated c_v is very low (0.17), suggesting that the service time distribution is likely to be a deterministic distribution. Indeed, the cumulative histogram obtained from the service time samples is similar to a step function with an inflexion point between 45 and 55 seconds (see Figure 5(a)), with a sample mean of 51 seconds. This differs slightly from the true value of 48 seconds, a deviation that is expected, since the case study was executed under human control with a slight delay when a customer finished being served and began to leave the server's service area.

The c_v of service time sample in Case Study 2 is very close to the actual value 1, which is the c_v of an exponential distribution. The results of all three goodness of fit tests (see Table 5) also accept that the null hypothesis that the service time sample is extracted from an exponential distribution. The estimated parameter of the best-fit exponential distribution is 0.02561 (cust/sec), which is close to the theoretical value 0.02833 (cust/sec), as shown in Figure 5(b).

The c_v of the service time samples in Case Study 3 (see Table 4) and the goodness of fit test results (see Table 5) all indicate that the service time is very likely to be sampled from an exponential distribution. However, the true service time distribution should be a hyper-exponential distribution with c_v around 1.5. From Figure 5(c), we can see that the shapes of the actual service time distribution

bution and the best-fit exponential distribution are very similar to each other. Given the limited size of the extracted samples, it is reasonable to make the statistical inference that the underlying distribution of the extracted service time sample is likely to be an exponential distribution with $\lambda = 0.0213$ cust/sec.

Case Study	c_v (estimated)	c_v (actual)
Case Study 1	0.89	1.00
Case Study 2	0.93	1.00
Case Study 3	0.87	1.00

Table 6: The coefficient of variation c_v of the extracted interarrival time samples compared to their actual values

Interarrival time

Table 6 shows the coefficients of variation calculated from the extracted interarrival time samples in the first three case studies. All of them are close to 1, which means that we infer the interarrival time samples are likely to be extracted from exponential distributions (which in fact they are).

Table 7 presents the results of applying three goodness of fit tests to the extracted interarrival time samples for the three case studies. The results show that the hypothesis that the underlying probability distribution of the sample is exponential cannot be rejected. It also compares the estimated λ of the best-fit exponential distribution with the actual values.

Routing Probabilities

path	count	nextFlow
Server1	27	Serverl
		Server2,
		Serverl
		Server3
Server2	1	
Server1 Server2	19	Serverl
		Server2
		Server3
Server1 Server3	4	
Server1 Server2 Server3	4	

Table 8: Customer flow analysis for Case Study 4

Table 8 shows the result of flow analysis (conducted in the fourth stage of the data processing pipeline) for Case Study 4. From the table, we can see that 19 out of 27 customers who completed service at Server1 went to Server2 for service and only 4 went to Server3 for service. In the actual setting, 70 percent of the customers go to Server2 and 30 percent of the customers go to Server3 after Server1. The experimental results differ from the actual probabilities because, as shown in Table 8, the flow analysis discovers some nonexistent paths, such as Server1 Server2 Server3 and Server2. This is due to the fact that some of the tags' locations were not updated regularly on account of the tags entering their "sleep" mode after being stationary for a period of time (Ubisense).

CONCLUSION AND SUMMARY

This paper has presented a four-stage data processing pipeline for extracting queueing models (specified in terms of routing probabilities, interarrival time distributions and service time distributions) from high-precision location tracking data. The pipeline gradually refines noisy low-level data (e.g. entities' Cartesian coordinates) into high-level historical traces of customer and server activities. From derived samples of customer interarrival times and service completion times, a simple workflow mining algorithm infers customer flow routing probabilities and fits arrival and service time distributions. These comprise a simple queueing network model of the monitored system made up of single-server nodes.

Through four case studies conducted in this project, the developed data processing method has shown moderate success in extracting performance models that display the true probabilistic features of the underlying system. The success is especially obvious with systems of lower levels of complexity and randomness.

In the future we intend to extend our methodology to support advanced features such as multiserver nodes, multiple classes of customer, customer priority schemes, and sophisticated arrival processes (e.g. correlated input traffic). We also wish to experiment with the application of such techniques in the context of real-life systems (e.g. healthcare environments).

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	Case Study 1		Case Study 2		Case Study 3		
	Kolmogorov-Smirnov		Kolmogorov-Smirnov		Kolmogorov-Smirnov		
test statistic	0	.1514	(0.068		0.0804	
α	0.1	0.05	0.1	0.05	0.1	0.05	
critical values	0.2109	0.2342	0.1538	0.1709	0.1257	0.1396	
rejected?	No	No	No	No	No	No	
	Anders	on-Darling	Anders	son-Darling	Anders	on-Darling	
test statistic	0	.8881	0.3704		0.7681		
α	0.1	0.05	0.1	0.05	0.1	0.05	
critical values	1.929	2.502	1.929	2.502	1.929	2.502	
rejected?	No	No	No	No	No	No	
	Chi	-squared	Chi	-squared	Chi	-squared	
test statistic		9.76		2.739		9.76	
α	0.1	0.05	0.1	0.05	0.1	0.05	
critical values	10.64	12.59	9.236	11.07	10.64	12.59	
rejected?	No	No	No	No	No	No	
estimated λ (cust/sec)	0.0195		0.01845		0.01715		
actual λ (cust/sec)	0.	01667	0.	02167	0.	01667	

Table 7: The results of three goodness of fit tests applied to the extracted interarrival time samples from three case studies. The null hypothesis is that the sample is from an exponential distribution. The estimated λ is the rate of the exponential distribution with the best fit to the sample data.

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Bond Graph Modelling and Simulation

GENERATING POSSIBLE CONFLICTS FROM BOND GRAPHS USING TEMPORAL CAUSAL GRAPHS

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KEYWORDS

Bond Graphs, Temporal Causal Graph, ARRs, Possible Conflicts, Model-based Diagnosis

ABSTRACT

Accurate modeling mechanisms play an important role in model-based diagnosis, and the bond graph modeling language has proved to be helpful for this task. In this paper we present an algorithm for automatically derive ARR-like structures, possible conflicts, from the bond graph model of a system. The algorithm uses temporal causal graphs as an intermediate structure to generate the set of possible conflicts. Performance of the algorithm for structural and sensor faults is then studied. Finally, we present another algorithm to automatically derive temporal information in the fault signature matrix for the set of possible conflicts, thus improving the isolation capabilities of the approach.

INTRODUCTION

Fault diagnosis and prognosis mechanisms play an important role in accurate and reliable operation of complex engineering systems. Accurate models play an important role in generating correct diagnosis results. Model-based reasoning approaches use the models as the core element for its reasoning process. Among all these approaches, model-based diagnosis techniques are becoming quite prevalent because of their generality, their applicability across multiple operating regions, and their potential for overcoming the device dependency problem.

An approach that has been successful for modeling the dynamic behavior of physical systems from first principles are bond graphs [Karnopp et al. (2000)]. Bond graphs provide an easy, intuitive way to build multi-domain energy-based models by combining system topology with a small set of component behavior processes. The topological structure of bond graph models also provides the infrastructure for developing effective and efficient fault diagnosis methods based on causal analysis that links component parameters to system variables using well defined methods.

Several approaches have been proposed to carry on the diagnosis process from bond graph models [Mosterman and Biswas (1999); Samantaray and Bouamama (2008)].

In earlier work [Bregon et al. (2008)], we compared some of these approaches against the possible conflicts diagnosis approach [Pulido and Alonso-González (2004)], an ARR-like compilation technique from the Artificial Intelligence Diagnosis (DX) community. In this work we showed the advantages of exploiting causal and temporal relations between process parameters and the measurement variables, provided by temporal causal graphs, for residual generation and analysis. The goal of this paper is to develop and automatic way to exploit these relations within the possible conflicts diagnosis framework.

Main contributions of the paper are as follows: (1) we developed an algorithm to automatically compute the set of possible conflicts for a system from its bond graph model using temporal causal graphs, i.e., minimal sets of equations that can be used for diagnosis purposes, (2) PCs and ARRs use different minimality concepts, the proposed algorithm allows to automatically generate the set of possible conflicts which include the set of structurally independent ARRs, but also additional PCs which can be used for sensor fault isolation, and (3) we propose an algorithm to automatically generate the fault signature matrix of the set of possible conflicts including temporal information.

The rest of the paper is organized as follows. The next section briefly describes the bond graph approach. A three tank system is used to illustrate the modeling approach. This is followed by a discussion of the possible conflicts approach to diagnosis. The following section presents the algorithm to automatically derive the set of possible conflicts from the bond graph model of a system. The basis for the possible conflicts' fault signature matrix generation with temporal information are presented. Next, results for the case study of a nonlinear, controlled three tank system are shown. Finally, the last section presents conclusions and future work.

BOND GRAPH MODELING

Bond graphs are labeled, directed graphs, that present a topological, domain-independent, energy-based methodology for modeling the dynamic behavior of physical systems [Karnopp et al. (2000); Samantaray and Bouamama (2008)]. Building system models follows an intuitive approach where energy flow paths between system components are captured by a topological structure

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where system components appear as nodes, and the energy flow paths appear as links or bonds. We will use the laboratory plant model of a three tank system (shown in fig. 1) to illustrate the significant concepts in this paper.



Figure 1: Three-tank system.

Fig. 2 shows the bond graph model for the plant. The tanks are modeled as capacitors that hold fluid, and the valves and pipes as resistances to flow. 0– and 1– junctions represent the common effort (i.e., pressure) and common flow (i.e., flowrate) points in the system, respectively. Measurement points, shown as De components, are connected to junctions, and the faults appear as explicit parameters of the bond graph model.



Figure 2: Bond graph model of the plant including the effort measurements $(De : P_1, De : P_2)$

This representation provides a systematic framework for capturing causal relations between system variables, i.e., causal graphs can easily be automatically derived from bond graph models. A special class of causal graph, is the Temporal Causal Graph, that captures not only the causal, but also the temporal relations between system variables.

Deriving Temporal and Causal Relations: the Temporal Causal Graph

Temporal Causal Graphs, TCG, defined by Mosterman and Biswas [Mosterman and Biswas (1999)] for diagnosis tasks, are an extended form of signal flow graphs for dynamic systems, that capture the causal and temporal relations between process parameters and the measurement variables in the system. More formally, a TCG can be defined as [Roychoudhury et al. (2006)]:

Definition 1 (Temporal Causal Graph). A TCG is a directed graph $\langle V, L, D \rangle$. $V = E \cup F$, where V is a set of vertices, E is a set of effort variables and F is a set of flow variables in the bond graph system model. L is the

label set $\{=, 1, -1, p, p^{-1}, pdt, p^{-1}dt\}$ (*p* is a parameter name of the physical system model). The *dt* specifier indicates a temporal edge relation, which implies that a vertex affects the derivative of its successor vertex across the temporal edge. $D \subseteq V \times L \times V$ is a set of edges [Narasimhan and Biswas (2007)].

TCGs can be directly derived from bond graph models, with effort and flow variables represented as vertices, and relations between the variables represented as directed edges.

Fig. 3 shows the TCG for the three tank system. Junctions and resistors define instantaneous magnitude relations, and capacitors and inertias define temporal effects on causal edges.



Figure 3: Temporal causal graph of the three tank system.

POSSIBLE CONFLICTS DIAGNOSIS APPROACH

Consistency based approaches are commonly employed in model-based diagnosis methods employed by the Artificial Intelligence community. Possible conflicts, PCs for short [Pulido and Alonso-González (2004)], are those sub-systems that may become conflicts when faults occur within the Consistency Based Diagnosis framework [Reiter (1987)], i.e., *minimal subsets of equations containing the analytical redundancy necessary to perform fault diagnosis* [Pulido and Alonso-González (2004)].

Computation of PCs is performed on an abstract model linked to the set of equations in the system description, i.e., a hypergraph including just the constrains in the model, and their related known and unknown variables. PCs are derived off-line using two core concepts: *minimal evaluation chains*, or MECs, and *minimal evaluation models*, or MEMs.

MECs are minimal over-constrained sets of relations, and they represent a necessary condition for a conflict to exist. MECs represent a partial subhypergraph from the original system description.

Each constraint in a MEC has one or more variables, and each variable could be solved using the constraint, assuming the remaining variables are known. This fact is called an interpretation for the constraint, i.e. a feasible causal assignment. In the general case, not every interpretation is feasible for non-linear dynamic models. The set of interpretations, seen as causal links among variables in each hyper-arc, define a causal graph for each MEC. A MEM is a global consistent causal interpretation for every constraint in a MEC. Hence, a MEM is a subgraph for each MEC. Using the whole set of available interpretations for each constraint in a MEC, algorithms used to compute PCs are able to find every possible causal interpretation which is globally consistent within a MEC, i.e., the whole set of MEMs for each MEC. Each MEM describes an executable model, which can be used to perform fault detection. Possible Conflicts are defined as the set of relations in a MEC that has, at least, one MEM.

If there is a discrepancy between predictions from these models and current observations, the PC must be responsible for such a discrepancy, and should be confirmed as a real conflict. Afterwards, diagnosis candidates are obtained from conflicts following Reiter's theory. Further information concerning PC calculation can be found in [Pulido and Alonso-González (2004)].

PCs calculation uses a minimality criteria in terms of sets of constraints. Nevertheless, it is straightforward to obtain candidates based on components. As pointed out in [Pulido and Alonso-González (2004)], the set of MEMs generated with this approach is equivalent to the set of conflicts computed by the GDE.

Moreover, if algorithms used to compute ARRs through structural analysis use such minimality criterion and provide a complete solution –explores every possible causal assignment for every minimal ARR–, the set of PCs has same detection and isolation capabilities as the set of minimal ARRs.

Finally, if every MEM in every PC provides the same solution–what is called the *Equivalence assumption* in [Pulido and Alonso-González (2004)]–, then PCs, minimal ARRs, and minimal conflicts provide the same solution in terms of fault detection and isolation capabilities.

Cordier et al. [Cordier et al. (2004)] introduced the concept of *support* for an ARR (set of components whose models are used to derive an ARR). Based on such idea, off-line compiled conflicts and ARR's support can be considered as equivalent (the support for an ARR is a potential conflict, which is equivalent to a possible conflict [Cordier et al. (2004); Pulido and Alonso-González (2004)]). Under given conditions, the set of minimal ARRs and the set of minimal conflicts will have same detection and isolation capabilities.

Once minimal PCs of a system have been identified, the next step deals with establishing the set of PCs that would be activated in presence of each fault, i.e., the fault signature matrix, FSM. The FSM relates faults that can occur in the system with PCs that would be activated for each fault.

For the three tank plant, two PCs are derived. Table 1 shows the resulting fault signature matrix. Columns PC_1 and PC_2 show the theoretical activation values of the PCs in presence of the different kind of faults considered (shown in the first column). Column I shows the

isolation capabilities of the approach.

	PC_1	PC_2	Ι
C_{T_1}	1	0	1
C_{T_2}	1	1	0
C_{T_3}	0	1	0
R_{V_1}	1	1	0
R_{V_2}	1	1	0
R_{V_3}	0	1	0

Table 1: Signature matrix of the possible conflicts found for the three tank system.

Current implementation of PCs computation needs the hypergraph and the interpretation for each hyper-arc to be provided by the user. In this work we employ the structural, causal and temporal information provided by the TCGs derived from the bond graphs, to automatically compute the set of PCs from a given system description. The only requirement is to have the system description as a bond graph.

PC DERIVATION FROM BOND GRAPHS

In this section we present an algorithm to automatically derive the set of PCs from the bond graph model of a system. Similar approaches have already been proposed in the literature for the same purpose. Samantaray et al. [Samantaray and Bouamama (2008); Samantaray et al. (2006)] introduced the Diagnostic Bond Graphs, DBG, as a way to obtain all the ARRs of a system. The problem with this approach is that it requires a previous process of causality inversion in the sensors, what makes it difficult to automate the whole process of ARR generation. Other approaches, like [Bouamama and Samantaray (2003)], present the steps that must be followed to generate the set of ARRs, but no algorithm is provided.

Moreover, as shown in [Bregon et al. (2008)], the PCs diagnosis approach exhibits some advantages against the ARRs approach. While ARRs/DBGs are designed to use derivative causality in the system [Samantaray and Bouamama (2008)], PCs are designed to automatically work with both integral or derivative causality. Another important difference is that ARRs consider that discrepancies in the system can only be found comparing an estimated variable against a measured one. PCs, on the other side, consider that discrepancies in the system are found comparing an estimated variable against a measured variable, or just comparing two variables that can be estimated by means of the measured ones.

To compute the set PCs we need to look for MECs with at least one MEM. MEMs can be derived while finding MECs, just checking global consistency of the causal graph w.r.t. the causal assignments. Temporal causal graphs are pretty suitable for this purpose, because are able to provide all the causal paths from a variable to the sensors or sources. Moreover, TCGs will provide the system with temporal information that, as we will see later, can be used to improve the isolation capabilities of the approach. Therefore, we will used TCGs as an intermediate step for PCs computation from bond graphs.

Algorithms to automatically derive the TCG from the bond graph model can be found in the literature [Mosterman and Biswas (1999)]. Once the TCG has been derived, we have to clearly mark the following items within the TCG model in order to derive MEMs:

- Sensors in the system, i.e, measured variables.
- Discrepancy nodes, i.e, measured, and nonmeasured variables in the TCG whose value can be estimated by two independent incident edges.

Algorithm 1 is invoked on the temporal causal graph to obtain the set of possible conflicts of the system. For every discrepancy node, this algorithm invokes algorithm 2. Algorithm 2, is a recursive algorithm that propagates backward along the directed edges of the temporal causal graph trying to eliminate all unknown variables from the discrepancy node. When all unknown variables are eliminated by means of measured variables ($vertex == \emptyset$), a PC has been found, and minimality conditions have to be checked. If the PC is minimal w.r.t. the rest of the PCs found in the system, the PC is added to the set of PCs, SPC; if not, the PC is discarded. An example of its application from the discrepancy node e_2 (that is measured and can also be estimated) is shown in fig. 4.

Algorithm 1: For each discrepancy node, dn, marked in the TCG, we try to find any possible conflict, pc; SPC is the set of possible conflicts; SDN is the set of discrepancy nodes

```
    function SPC := find_every_pc_foreach_dn (SDN)
    foreach dn in SDN do
    vertex = {dn};
    find_pc(vertex, {}, SPC)
    end
```



Figure 4: PC_1 derivation by means of algorithm 2 for find_pc($\{e_2\}, \{\}, SPC$)

Looking at the TCG for the running example (fig. 2) the reader can see that a PC can be obtained propagating backwards through the TCG from the discrepancy node e_2 . The backward propagation will stop when all the unknown variables become explained. In this example, when the backward propagation reaches the measured variable e_{11} , the algorithm will stop and identify a possible conflict (see figure 4). Another PC can be found propagating backwards in the TCG from the discrepancy node

Algorithm 2:

1	function find_pc (vertex, pc, SPC)
2	if $vertex == \emptyset$ then
3	if pc is not in SPC and pc is minimal then
4	insert pc in SPC ;
5	end
6	else
7	foreach v' in vertex do
8	$vertex = vertex \setminus \{v'\};$
9	foreach ancestor vertice av' needed to compute
	v' do
10	if av' has not been visited then
11	if av' is a source or a sensor then
12	$pc = pc \cup \{av'\};$
13	else
14	$vertex = vertex \cup \{av'\};$
	$pc = pc \cup \{av'\};$
15	end
16	end
17	find_pc(vertex, pc, SPC);
18	end
19	end
20	end

 e_{11} until the measured variable e_2 is reached. To find both PCs, we have considered the observational model of the system implicitly included in the TCG, i.e., e_2 and e_{11} are directly marked as measured variables. But, what happens when the observational model is explicitly included in the TCG?.

Extension to Sensor Faults

As Bouamama et al. claim [Bouamama and Samantaray (2003)], in presence of multiple sensors, if some residuals share common variables, linear combinations of these residuals can produce independent residuals. Although it is quite clear that these residuals cannot provide additional structural isolation capabilities to the diagnosis system, they can be used for sensor fault isolation. One of the advantages of the proposed algorithms is that just slight changes in the TCG need to be made:

 TCG have to be modified in such a way that the observational model of the system becomes explicitally included.

For the three tank running example, sensor variables s_1 and s_2 have to be included in the TCG. Now, variables e_2 and e_{11} could be either estimated or measured. Fig 5 shows the extended TCG for the three tank system example.

Following with the three tank running example, if we invoke algorithms 1 and 2 on the extended TCG (fig. 5) from the discrepancy node e_2 , we obtain: (1), the same PC that we previously obtained (PC_1) if the path from e_{11} to the sensor s_2 is followed (see upper part of fig. 6); and (2), a new PC if the path from e_{11} to the variable f_{11} (and further backward propagation) is followed (see lower part of fig. 6). In terms of minimality criteria,



Figure 5: Extended temporal causal graph of the three tank system.

the new PC will be minimal w.r.t the other PC because now we are considering sensor equations as part of the system, and consequently, the new PC is not maximal from the already existing PC (because does not include the sensor equation).





Figure 6: PC_1 (upper part) and additional PC_3 (lower part) for the first sensor obtained using the modified algorithm 2. PC_1 explains the variable e_{11} propagating backwards through the edge to the measured variable s_2 . The additional PC_3 explains the variable e_{11} propagating backwards through the edge to the variable f_{11} .

Table 2 shows the resulting signature matrix for the extended version of the algorithm. Columns show the theoretical activation values of the PCs in presence of the different kind of faults considered (shown in the first column). Columns PC_1 and PC_2 show the original PCs found in the system (also found with the new version of the algorithm). Column I_1 shows the isolation capabilities these two PCs. Columns PC_3 and PC_4 show the additional PCs obtained for the system, and column I_2 shows the isolation capabilities of the approach for the whole set of PCs. Additional rows have been added to the FSM for each of the sensor faults considered. Looking at columns I_1 and I_2 , it is clear that using the original set of PCs, sensor faults cannot be isolated, but if the whole set of PCs is used, both sensor faults can be isolated.

	PC_1	PC_2	I_1	PC_3	PC_4	I_2
C_{T_1}	1	0	1	1	1	1
C_{T_2}	1	1	0	1	1	0
C_{T_3}	0	1	0	1	1	0
R_{V_1}	1	1	0	1	1	0
R_{V_2}	1	1	0	1	1	0
R_{V_3}	0	1	0	1	1	0
S_1	1	1	0	1	0	1
S_2	1	1	0	0	1	1

Table 2: Signature matrix for the whole set of possible conflicts found for the three-tanks system.

THE REDUCED QUALITATIVE FAULT SIGNA-TURE MATRIX

Given current observations, residual for PCs and ARRs, should provide values in presence of the different kind of faults as 1 if the residual is activated, or 0 if it is not activated. Recently, several authors [Koscielny (1995); Koscielny and Zakroczymski (2000); Puig et al. (2005); Gelso et al. (2008)] have proposed extensions to improve the fault detection and isolation stages based on ARRs or PCs, including temporal information about residuals. The problem is that such extensions are hard to obtain automatically.

The qualitative fault signatures approach from Mosterman and Biswas [Mosterman and Biswas (1999)] uses the properties of TCGs to automatically derive the FSM of a system including temporal information (known as the qualitative fault signature matrix, QFSM). Given a set of faulty parameters and a set of measurements associated with a system, the qualitative fault signatures can be derived from the TCG model of the system by forward propagation from the fault parameter along the edges of the TCG to the measurement nodes [Mosterman and Biswas (1999)].

Our proposal consists in applying a TRANSCENDlike forward propagation algorithm to automatically obtain the qualitative fault signature matrix for each of the PCs of a system. As we used the TCG to generate the set of PCs, we can now use the TCG model of each PC to propagate forward from the fault parameter along the edges to the discrepancy nodes of the PCs to obtain a FSM with temporal information. We will call this matrix, the reduced qualitative fault signature matrix (RQFSM).

The method for predicting future behavior is shown in algorithm 3. The algorithm uses the TCG model of each PC to find the signatures. For each hypothesized fault that can activate a PC, the algorithm invokes TRANSCEND's prediction algorithm [Mosterman and Biswas (1999)] using only the TCG model of the PC. This prediction algorithm [Mosterman and Biswas (1999)] will compute, in a qualitative way, the behavior of the discrepancy nodes of the PCs, i.e., the behavior of the PC. This behavior is expressed in terms of the magnitude (zeroth order time-derivative), slope (first order time-derivative), and higher order effects. All deviation propagations start off as zeroth order effects (magnitude changes). When an integrating edge in the TCG is traversed, the magnitude change becomes a first order change, i.e., the first derivative of the affected quantity changes.

Algorithm 3: F	or each possible	conflict's TCG,
TCG_{PC_X} , we fi	nd the signatures	for all hypothe-
sized faults using	a TRANSCEND-1	ike prediction al-
gorithm; SPC is the	ne set of possible c	conflicts
gorithm; SPC is the	ne set of possible c	conflicts

1	<pre>function RQFSM := find_rqfsm(SPC)</pre>
2	foreach PC_X in SPC do
3	foreach fault candidate in PC_X do
4	Predict_Future_Behavior _Algorithm(TCG_{PC_X} ,
	fault candidate)
5	end
6	end

Algorithm 3 returns the signature of all hypothesized fault for each PC. It is important to point out that TRAN-SCEND's algorithm can not be directly used to get the RQFSM of a system, because the algorithm has to be invoked as many times as PCs have been found in the system, and for the parts of the TCG related with the PCs.

Table 3 shows the reduced qualitative fault signature matrix for the three tank plant. Columns PC_1 and PC_2 represent the expected deviations (no change (0), or increasing or decreasing (+/-)) in the magnitudes, and in the slope or higher order effects, in the presence of faults for each possible conflict. Column *I* shows isolation capabilities of this approach. Column *I* clearly shows the increment in the discrimination power compared with previous approaches, due to the inclusion of temporal information (in magnitudes, slopes and higher order effects) in the theoretical FSM.

	PC_1	PC_2	Ι
C_{T_1}	-+		1
C_{T_2}	0-	0-	1
C_{T_3}		+-	1
R_{V_1}	0+	0-	0
R_{V_2}	0+	0-	0
R_{V_2}		0+	1

Table 3: RQFSM found for the three tank system.

CASE STUDY

The laboratory plant shown in fig. 7 will be used to study the proposed algorithms. This plant resembles common features of a continuous industrial process. It is made up of three tanks $\{T_1, T_2, T_3\}$. A control loop defined by a function f(x), where x is the pressure in tank T_1 , determines the opening of valve V_0 . Valves V_1, V_2 , and V_3 are completely open. We assume four sensors: two, $\{P_1, P_2\}$, measure the fluid pressure in tanks T_1 and T_3 , the third, $\{F_1\}$, measures the in-flow into tank T_1 , and the fourth, $\{F_2\}$, measures the outflow from tank T_3 . For this study, we consider seven different parametric faults in the plant: change in tanks T_1, T_2, T_3 capacities, and block in valves V_1 , V_2 , V_3 , and in the input pipe. We also consider sensor faults.



Figure 7: Diagram of the laboratory plant.

Fig. 8 shows the bond graph model for the plant. Measurement points shown as De and Df components are connected to junctions, and the faults listed above, appear as explicit parameters of the bond graph model. Fig. 9 shows the TCG for the plant.



Figure 8: Bond graph model of the plant. Here, f(x) represents the function of the pressure in T_1 that controls the resistance R_{valve} (control on the aperture of V_0).

Results for the Case Study

Invoking algorithms 1 and 2 from the three tank plant's TCG we automatically obtained a set of four possible conflicts. Table 4 shows the FSM for this set of PCs. Columns PC_1 , PC_2 , PC_3 , and PC_4 show the theoretical activation values of the PCs in presence of the different kind of faults considered (shown in the first column). Column I shows the isolation capabilities of the approach. Results for this plant are equivalent to those obtained using the the ARR/DBG approach for the same model (as stated in [Bregon et al. (2008)]).

	PC_1	PC_2	PC_3	PC_4	Ι
C_{T_1}	0	1	0	0	1
C_{T_2}	0	1	1	0	0
C_{T_3}	0	0	1	0	1
R_{V_1}	0	1	1	0	0
R_{V_2}	0	1	1	0	0
R_{V_3}	0	0	0	1	1
R_{nine}	1	0	0	0	1

Table 4: Signature matrix of the possible conflicts found for the laboratory plant.

If sensor faults are considered, we can invoke the extended version of algorithm 2. With this approach, we obtained a set of 15 minimal PCs for the system. Table 5 shows the fault signature matrix for these 15 PCs.



	PC_1	PC_2	PC_3	PC_4	I_1	PC_5	PC_6	PC_7	PC_8	PC_9	PC_{10}	PC_{11}	PC_{12}	PC_{13}	PC_{14}	PC_{15}	I_2
C_{T_1}	0	1	0	0	1	1	1	1	1	1	1	1	1	1	0	0	1
C_{T_2}	0	1	1	0	0	1	1	1	1	1	1	1	1	1	1	1	0
C_{T_3}	0	0	1	0	1	0	1	0	1	1	1	1	1	1	1	1	1
R_{V_1}	0	1	1	0	0	1	1	1	1	1	1	1	1	1	1	1	0
R_{V_2}	0	1	1	0	0	1	1	1	1	1	1	1	1	1	1	1	0
R_{V_3}	0	0	0	1	1	0	0	0	0	0	1	1	0	1	1	1	1
R_{pipe}	1	0	0	0	1	1	1	1	1	1	1	1	0	0	0	0	1
F_1	1	1	0	0	0	1	1	0	0	0	0	0	1	1	0	0	1
P_1	1	1	0	0	0	0	0	1	1	0	0	0	1	0	1	1	1
P_2	0	1	1	1	1	1	0	1	0	1	1	0	0	1	1	0	1
F_2	0	0	1	1	1	0	1	0	1	1	0	1	1	0	0	1	1

Figure 9: Temporal causal graph of the three tank plant.

Table 5: Signature matrix for the whole set of possible conflicts found for the laboratory plant.

Columns PC_1 to PC_4 show the results for the four initial PCs previously obtained. Column I_1 shows the isolation capabilities of first four PCs. Columns PC_5 to PC_{15} show the additional PCs obtained for the system, and column I_2 shows the isolation capabilities of the approach for the whole set of PCs. Additional rows have been added to the FSM for each of the sensor faults considered. Looking at columns I_1 and I_2 , it is clear that fault discriminability for sensor faults is increased with the new set of additional PCs.

Finally, invoking algorithm 3 we automatically obtain the reduced qualitative fault signature matrix for the plant (see table 6). In this table, columns PC_1 to PC_4 represent the expected deviations (no change (0), or increasing or decreasing (+/-)) in the magnitudes, and in the slope or higher order effects, in the presence of faults. Column I shows isolation capabilities of this approach. For the sake of simplicity we only show the results obtained for the initial set of four PCs and only for parametric faults.

	PC_1	PC_2	PC_3	PC_4	Ι
C_{T_1}		+*			1
C_{T_2}		0+	0+		1
C_{T_3}			+-		1
R_{V_1}		0-	0+		0
R_{V_2}		0-	0+		0
R_{V_3}				+-	1
R_{pipe}	+*				1

Table 6: RQFSM found for the laboratory plant.

Comparing tables 4 and 6 it is clear that the RQFSM is better for isolation purposes. A fault in C_{T_2} can now be isolated from a fault in R_{V_1} or R_{V_2} due to the sign in

the derivative. The great advantage of this approach is that using algorithm 3 the RQFSM can be automatically computed for PCs.

CONCLUSIONS AND FUTURE WORK

In this paper, we have presented an algorithm to automatically compute the set of possible conflicts for a system from its bond graph model. Using the causal structure implied by the topological structure of the bond graph models (obtained through temporal causal graph models that can be automatically derived) greatly facilitates the possible conflicts generation process, because the structure of each PC can be seen as equivalent to a minimal subset of over-determined equations within the TCG, i.e, PCs identify minimal structures in TCGs [Bregon et al. (2008)]

We have proved that explicit inclusion of the observational model of the system in the TCG can lead to additional possible conflicts generation. These possible conflicts does not improve discrimination capabilities of the PCs approach but have proved to be useful to discriminate sensor faults. The proposed algorithms are able to work with this extended TCG and automatically compute the whole set of additional possible conflicts.

Finally, using the temporal relations established in the temporal causal graph, we have proposed an algorithm to compute an extended version of the fault signature matrix for the diagnosis system. This new fault signature matrix, called reduced qualitative fault signature matrix, includes information about the sign in the magnitudes, slopes, and higher order effects. This new fault signature matrix improves diagnosability of the diagnosis approach for structural faults.

In future work, we will extend our algorithms to compute the set of possible conflicts from hybrid bond graph models. We will also try to test the approach in different and more complex forms of nonlinear systems.

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Bond Graph based control of a three phase inverter with LC filter

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Bond Graph, inverter.

ABSTRACT

In this paper is proposed a model of a three phase electrical inverter with a LC output filter in delta connection used in a renewable energy supply system. The concept of inverse bond graph via bicausality is used for the control law design. The control law is compared in simulation with another traditional one and validated experimentally.

INTRODUCTION

Power systems have been developed over the years to supply a varying demand from centralized generation sources of fossil and nuclear fuels. Nowadays the renewable energy sources start to play an important role in the grid connection, so the renewable sources need to be integrated into the electrical network via electronic power converters.

The electronic power converters are not only used for the connection between a renewable energy source and the network, they are also used in many industrial applications. The multi physics aspect of such systems justifies the bond graph approach.

The bond graph model of a three phase inverter has been addressed in several research papers, as for example for the most recent publications: [Mezghanni et al., 2007; Belhadj, 2006; González-Contreras et al., 2007]. Each presented model has different characteristics and is used for different applications. They have in common that they have been established

with an electronic switch (MTF) for modeling the

commutation cell of the converter; moreover the different papers used a PWM technique for controlling the commutations in these elements. Here we propose to model the three phase electrical inverter with only two electronic switches [Guillaud & Francois, 2003] and to control it without using PWM method.

For designing the control law, we use the inverse bond graph model using the bicausality concept [Ngwompo et al, 1996]

A specific controller is proposed combining the inverse model and a resonant block.

The outline of this paper follows. In the second section a presentation of the global system is given. In section 3 the bond graph model of a three phase inverter with LC filter is proposed and some causality problems are discussed. A two stage control law for the inverter is given in section 4. Section 5 shows the experimental and simulation results. Finally some conclusions are given.

PRESENTATION OF THE GLOBAL SYSTEM

Figure 1 shows the global scheme of a renewable energy source connected to a load. This structure is the basic one and could be analyzed at different levels of complexity.

The renewable energy source could be a panel of photovoltaic cells, a gas turbine or a wind turbine. It delivers the primary power in the DC bus which will be converted into AC power via the power converter. The introduction of a capacitor on the DC bus is necessary in order to have a decoupling between the harmonics generated by both converters. In this part of the system, it is necessary to make the regulation of voltage (u_s) or current (i_m) .



Figure 1 Global electrical system.

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) The power electronic converter might be considered as an amplifier. It is composed of three pairs of electronic switches (Mosfet, IGBT, etc.). Each pair of switches is called a commutation cell.

In the filter part, the basic one is known as a LR filter, which consists only in one inductance in series with a resistance; it can be taken as a base for more complex filters, only by adding more components, for example LC one (figure 1) which has one inductance and resistance in series with a capacitor in parallel. Each filter configuration has its own characteristics and is used for specific requirements or analysis from the point of view of stability and harmonics analysis.

In figure 1, the currents in inductances L_{si} , i=1, 2, 3, and the voltages of capacitors C_1 , C_2 , C_{12} are controlled. Thus, the behavior of this system may be assimilated to a voltage source, contrary to the classical LR filter structure which is assimilated to a current source. The main advantage with such a voltage source is in case of connection to the grid, because it avoids any dependence of the voltage in the C-elements to the voltage grid.

The grid will be chosen here as a passive load (R, L).

MODEL OF THE INVERTER AND THE FILTER

In this paper the model of the inverter shows up explicitly only two of the three commutation cells, the third one fixing the voltage reference. Only 2 phase to phase voltages (u_{m1}, u_{m2}) have to be considered for control [Guillaud & Francois, 2003]. The current i_{s3} is linearly dependent of the two others $(i_{s1} \text{ and } i_{s2})$.

We are focusing on the average behavior of the converter. Furthermore, we are not interested in the switches themselves, but on the impact of the converter on the LC filter.

Thus, we define 2 control signals (m_1, m_2) which are defined as:

$$m_1 = \frac{u_{m1}}{u_s}$$
 and $m_2 = \frac{u_{m2}}{u_s}$ (1)

The primary source of the converter in the DC bus is represented as a constant voltage source (u_s) by assuming that it has no variation or fluctuation.

The three phase LC filter is composed of three inductances with their associated resistance and three Delta connected capacitors.

The model is made in two stages. Firstly, the three inductances and their associated resistances are taken into consideration; secondly the three capacitors are added.

The three phase inverter model with the LR filter is shown figure 2. The element I: L_{s3} has a derivative causality because of the 0-junction placed between the bonds 21, 22 and 23, which represents the Kirchhoff law (sum of the currents equal to zero).



Figure 2 Bond Graph model of the three phase inverter with a LR filter.

Taking the bond graph of figure 2 as base, the three C-elements are added (figure 3).



Figure 3 Bond Graph model of the three phase inverter with a LC filter.

In figure 3 the element C: C_{12} has a derivative causality because of the 1- junction linking bonds 24, 25 and 26, which represents the Kirchhoff law (sum of the voltages equal to zero).

The bond graph model shows up two causality loops (following effort and following flow) in bonds 24, 26, 14, 12, and two others in bonds 25, 26, 20, 18 [Van Dijk & Breedveld, 1991], each of them with a gain equal to minus one. Thus, the model can be simulated. These causality loops are introduced because of the configuration in Delta connection of the capacitors. In a star connection they would not exist.

The bond graph model explicitly points, out the physical insight of the system with the two elements in derivative causality (L_{s3} and C_{12}).

Finally, figure 4 shows the connection of L-R elements (load) for each branch.



Figure 4 Bond Graph model with the connection of a load.

Elements L and R in bonds 24, 25 and 26 are assigned with integral causality.

The four detectors (Df: i_{s1} , Df: i_{s2} , De: u_{c1} , De: u_{c2} ,) shown in figure 4 are associated with the sensors.

CONTROL OF THE INVERTER AND THE FILTER

In this section we propose a new control structure for the three phase converter, and we recall a classical one which will be used for comparison purpose.

Control via inverse model and bi-causality bond graph

The control law applied to the model is based on the bicausality bond graph, and is designed from the inverse bond graph.

The notion of bicausality was introduced by Gawthrop [Gawthrop, 1995], and can be used to point out properties about inverse dynamics [Ngwompo et al, 1996] and parameter estimation [Ngwompo & Scavarda, 1999].

For the formulation of the inverse bond graph, it is necessary to change the flow detectors Df (supposed ideal) of the original bond graph for sources (named Se₀Sf, because they impose to the inverse model zero effort-non null flow), then propagate the bicausality (in only one line of power transfer) from this source (SS) to the input source of the original bond graph which becomes a detector in the inverse bond graph [Ngwompo et al, 1996].

With the inverse bond graph we design the structure of the control in open loop, which is then extended to a closed loop control by fixing the dynamics of the errors. The three phase voltages have to be controlled. However, there are two different ways to proceed:

- The first way assumes that the dynamics in the I: L_{si} elements are faster, compared with the dynamics in the C-elements. Thus only the voltages in C_1 and C_2 are controlled in closed loop; the voltage in the dependent C_{12} element is directly related to the two others.

- The other way considers the two loops in cascade, one for the current in the L_{si} and another one for the voltage in C_i -elements. In this paper, we choose to make the

control law via the two closed loops, for performance purpose.

The calculation of the control laws in the model is made in two steps, the first one for the currents and the next one for the voltages.

The figure 5 shows up the inverse bond graph, which allows deducing the open loop current control law. The two current sensors are inverted simultaneously via bicausal bonds and two disjoint bicausal paths are drawn to the two desired inverse model outputs corresponding to the two control signals (m_1, m_2) , which proves that the model is invertible [Ngwompo et al, 1996].



Figure 5 Inverse bond graph for the calculation of the current control law.

The I-elements are in derivative causality. Equation (2) is derived from the inverse bicausal bond graph of figure 5, by setting that the numerical values of R_{si} and L_{si} are the same for the 3 phases. It gives:

$$\binom{m_1}{m_2} = \left(\frac{1}{u_s}\right) \left(R_s + L_s \frac{d}{dt} \right) \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} i_{s1} \\ i_{s2} \end{pmatrix} + \begin{pmatrix} u_{c1} \\ u_{c2} \end{pmatrix}$$
(2)

For establishing the closed loop control law, we set up the dynamics of the error $(\varepsilon_i = i_{sref_i} - i_{s_i})$ in both expressions, as $\dot{\varepsilon}_i + k_{p1}\varepsilon_i = 0$, where k_{p1} is a constant gain to be fixed. The expression (2) becomes (3) as

$$\binom{m_1}{m_2} = \left(\frac{1}{u_s}\right) \left(\binom{R_s + L_s \frac{d}{dt}}{1} \binom{2}{1} \frac{1}{2} \binom{i_{slref} - \varepsilon_1}{i_{s2ref} - \varepsilon_2} + \binom{u_{c1}}{u_{c2}} \right) (3)$$

Finally,

$$\binom{m_1}{m_2} = \left(\frac{1}{u_s}\right) \binom{2}{1} \binom{2}{2} R_s \binom{i_{s1}}{i_{s2}} + L_s \frac{d}{dt} \binom{i_{s1ref}}{i_{s2ref}} + k_{p1} \binom{i_{s1ref}-i_{s1}}{i_{s2ref}-i_{s2}} + \binom{u_{c1}}{u_{c2}} \end{pmatrix}$$
(4)

As for the determination of the current control, the voltage control law is calculated; it provides the current reference for equation (4). Figure 6 shows the inverse

bond graph used for the determination of the current reference.



Figure 6 Inverse Bond Graph for the voltage control law.

For deriving equation (5) from figure 6, we follow the same procedure as previously. Two bicausal disjoint paths exist from one $SeSf_0$ to one De_0Df . The model is thus invertible. It leads to

$$i_{s_{1}ref} = C \frac{d}{dt} (2u_{c_{1}} - u_{c_{2}}) + i_{r_{1}}$$

$$i_{s_{2}ref} = C \frac{d}{dt} (2u_{c_{2}} - u_{c_{1}}) + i_{r_{2}}$$
(5)

According to the fact that the 3 capacitors are supposed with the same values capacitances, thus equations (6) show up the voltage control law for the converter.

$$\begin{pmatrix} i_{slref} \\ i_{s2ref} \end{pmatrix} = \begin{pmatrix} 2 & -l \\ -l & 2 \end{pmatrix} \begin{pmatrix} C\frac{d}{dl} \begin{pmatrix} u_{clref} \\ u_{c2ref} \end{pmatrix} + Ck_{p2} \begin{pmatrix} u_{clref} - u_{c1} \\ u_{c2ref} - u_{c2} \end{pmatrix} \end{pmatrix} + \begin{pmatrix} i_{r1} \\ i_{r2} \end{pmatrix} (6)$$

In equations (4) and (6), k_{p1} and k_{p2} are constant gains to be fixed. We choose to change k_{p2} for a resonant controller given equation (7) [Sato et al., 1998; Guillaud et al., 1999]:

$$\left(\frac{n_2 s^2 + n_1 s + n_0}{s^2 + \omega_n^2}\right) \tag{7}$$

In (7), the natural frequency (ω_n) is adjusted to the input signal frequency in order to obtain an infinite open loop gain at this frequency [Lopez de Heredia et al., 2006].

The calculation of the parameters in the resonant controller is made using the pole placement approach [Leclercq, 2004].

On the other hand, the gain k_{pl} is calculated for each phase by placing the pole of the polynomial denominator of the transfer function in closed loop derived from Figure 7. The desired performances for the closed loop model are given hereafter.



Figure 7 Block diagram for the current loop.

In figure 7, elements \hat{L} and \hat{R} are estimated values of the actual system parameters.

The controller block diagram of the complete model is shown in figure 8. It is important to notice that the structure of the control law contains a feed-forward with a derivative action on the references. The reference signals are sinusoidal and they can be derived analytically without any problem. The proposed control law is compared by simulation with a classical one described hereafter.

Control via Park transformation

A classical control approach consists in transforming the sinusoidal reference into a continuous reference by applying a framework change using the Park transformation. By this way, a classical proportional integral controller can be used without any problem, the resonant controller having no meaning here because of the constant value of the reference signals. As for the control previously presented, the control via Park transformation uses the two loop cascade control structure. Figure 9 shows the structure of the controllers.



Figure 8 Inverse model Controller block diagram in sinusoidal reference.



r igure 9 i i controller block diagram in i ark reference.

Simulation and experimental results of the two systems are shown in next section.

EXPERIMENTAL AND SIMULATION RESULTS

a) Simulation

The simulation results are obtained with the software 20Sim ®.

The table 1 shows the numerical values used in the model.

Table 1 Numerical parameters for the system	n and
control.	

System
$L_s = 0.55 mH R_s = 0.22 \Omega C = 22 \mu F R_r = 645 \Omega$
Values for inverse control law
$\hat{L}_s = 0.5mH \hat{R}_s = 0.2\Omega \hat{C} = 20\mu F$
$n_2 = 0.072 \ n_1 = 43.2 \ n_0 = 11009 \ k_{p1} = 2000$
Values for Park control law
$k_{p1} = 2.425 T_{p1} = 2.46e - 4 k_{p2} = 0.0336 T_{p2} = 1.2e - 3$

For the two models the references are two sinusoidal signals with 340 volts amplitude and 50Hz frequency, diphased of 120°.

The numerical values of table 1 have been calculated taking a time response of 10 ms in the voltage loops and 1 ms in the current ones.

Figures 10 and 11 show the simulation responses in one phase for the two closed loop models, when one step load change is made at time = 0.544 s. The load is balanced (same L and R parameter values in the three phases).



In figure 10, no change appears in the voltages. In the opposite, the figure 11 shows the change in the filter current responses.



Finally, in figure 12 is presented the load current.



We obtain the same responses in both control structures because the same time response has been considered. Consider now the case of an unbalanced load (third phase L and R parameter values different from the two others). Figure 13 shows the responses obtained for the control law with PI controllers in Park reference, and figure 14 for the responses from the proposed inverse model controller.







It is shown that the inverse model control has a better behavior compared to the PI one in the Park reference. Experimental implementation (as shown hereafter) confirms the robustness of the proposed new control law versus parameter uncertainties.

b) Experimentation

For the experimental implementation, we used a real time simulator as shown figure 15.



Figure 15 Scheme of the experimental set up.

The capacitor voltages (v_1, v_2, v_3) are transmitted to the high bandwidth power amplifier which applies the voltages to the load.

The currents flowing into the load are measured and introduced in the real time simulation model via an ADC (analogical to digital converter). The effect of the load is introduced in the real time simulator as a three phased current source.

For the experimental results, we considered the same numerical values as for the simulation (table 1).

We show up the responses for the voltage and currents for a LR series load. The reference voltage is 240 volts RMS and a three phase resistive load of 645 Ω with unbalanced inductances (0.1H, 0.107H and 0.08H). We applied one step change in the 3 R values (120 Ω) at 0.054 seconds. The three phase voltages are shown in figure 16.



Figure 16 Three phase voltage response for an unbalanced RL load.

As expected, we can notice in the figure 16 that the change in the load has no impact on the voltages. In the opposite, the actual change can be seen in the three load currents (figure 17).



Figure 17 Responses of the currents for an unbalanced RL load – step change in load R values at 0.054s

The unbalancing of the load due to a different value of the inductance in the phase 1 appears explicitly. In addition, for the filter currents (figure 18) we can notice a little change in the magnitude at time 0.054s. The perturbations in the signals are due to measurement noises.



unbalanced RL load.

The experimental results have been compared with the simulation results and we found that they are very similar.

CONCLUSIONS

A new bond graph model of a three phase inverter coupled with a LRC filter has been proposed. This model keeps the three branches of the AC current side and uses only two elements for the commutation of the inverter. Moreover, we proposed a new structure for the control law derived from the inverse bond graph using the concept of bicausal bond graphs. It has been shown through simulation and experimentation that the proposed control structure is robust versus parameter deviations.

The future developments will consist in connecting active loads to the system, such as an asynchronous machine.

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Electrical and Electromechanical Engineering

CONVERGED NEXT GENERATION NETWORK ARCHITECTURE & ITS RELIABILITY

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Abstract

The Next Generation Network is a future based network providing next generation services such as IPTV, Online gaming, Video on demand etc, based on IP protocol in the presence of core network. This research based Paper discusses the architecture of Next Generation Network, its challenges & solutions, its reliability and its pros & cons. The main objective is to investigate the effectiveness of NGN providing next generation services. This paper discusses the basic customers' needs and future trends of technologies perspective. Different technologies and their uses providing different services were reviewed. The term Next Generation Network (NGN) is used to support telecommunication network architecture and its technologies and services. Conventional Public Switched Telephone Network (PSTN) data, Voice Communication and Video Services are to be supported on the basis of NGN. The information carried through this network is based on packet switched form known as Internet network.

Keywords: SNMP, NGN, IPTV, Mobile, PSTN, Architecture, Packets, WiMax, Technology.

1. Introduction

1.1 Historical Perspective

With the development of new telecommunication technology, networks are becoming bigger and more complex. In the early 1980s, a tremendous change in the network deployment occurred in order to fulfil the requirement of customer needs and market trends. With the trend analysis and cost benefits, existing companies started to expand the network into large networks to get productivity gain and benefits [2]. In the mid-1980s, certain telecommunication companies felt frustration with existing networks which were incompatible with the other network technologies. The problems of network growth planning strategy and network operation management were associated in the development of network expansion. Every new deployed network requires its own set of functions and experts. Staffing requirement was an important factor to manage complex and network heterogeneous networks without а management system. This issue caused for

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) development of an automated network planning strategy and network management tools across a heterogeneous and complex network environment [1].

1.2 Definition of Technology

Technology progresses with the passage of time and trends. It is an application of knowledge to meet the demand of customer needs and goals. For example, fibre optic cables use single wavelength to carry hundreds of telephone conversations. Technology made it possible for the same fibre optic to carry a significant amount of information through Dense Wave Division Multiplex (DWDM) [2]. Many time signals are to be combined on the same fibre optic cable to carry much information by utilising different colour combinations of light.

The development of faster processors made it easier for software engineer to develop high-level languages like Java and many useful tools. The creation of useful tools and high-level programming languages made it possible for the development of complex and heterogeneous systems. There are following different technologies such as circuit switched, packet switched, intelligent networks, mobile networks, access technologies and voice and data convergence are used for the development of next generation network [2]. Now, these different technologies are described briefly such as:

1.2.1 Mobile Next Generation Networks

Future trends in telecommunications are going to be changed with the development of new technologies and services. Mobile Next Generation Networks played a pivotal role to reach the goal of truly ubiquitous computing [3]. The changed wired telephony services into database services, changed homogenous networks into complex heterogeneous network, changed non-intelligent devices into personal digital assistants and mobile computers created a big threat for the network service provider to accommodate the customer's needs and market trends [3].

Here, Diagram No. 1 shows the architecture of a mobile next generation network providing the wireless services with better coverage, signal strength, line of sight (LOS) etc. In Diagram No. 2, the architecture of WiMax is shown as a Mobile Next Generation Network. WiMax is a high speed wireless network providing a line of sight (LOS) better coverage and best signal strength as compared to other wireless technologies.



Figure 1. Architecture of Mobile Next Generation Network (WiMax) Source: WiMax Forum Aug (2006).



Figure 2. Architecture of Mobile Network

1.2.2 WAN Technologies

A Wide Area Network (WAN) allows the information travelling for longer distances and encounters a variety of physical and logical environments as compared to local area network (LAN). It involves 56 Kbps circuits, ISDN, leased

lines and frame relays for transformation of information over longer distances as comparatively local area networks.

In the diagram below, architecture of wide area network is depicted with the help of different network devices as shown:



Figure 3. Wide Area Network Architecture

1.2.3 Internet Technologies

Another emerging technology named as internet technology consists of different gateways, routers,

servers and different corporate LANS providing different services and technologies etc. Internet technologies or related networks run on an Internet Protocol (IP).



Figure 4. Internet Technologies Architecture
1.3 New wave of Services

At present, a new wave of services is emerging in order to satisfy customer needs and to ensure better services with current market trends. Currently, TV, PDA, Smart phone and PC-based browser are being used by next generation services driven by capacityintensive content that is being delivered by them [4].

Despite various content sources, commonality of these rapidly evolving services is IP-based [4]. These emerging services are, for example, IPTV for broadcast TV, Video on Demand (VOD), and Voice over IP (VOIP) for telephony and IP VPN for accessing corporate intranet. The other future based services like Over IP Video (OIPV), streamlining demanded video used by mobile devices, Games on Demand and network-hosted Personal Video Recorders (nPVR) are used for the personalized content delivery and storage etc [4]. To capture voice or video for subscription purposes or location aware service, VOD casting and POD casting are to be used.

"From a competitive standpoint, it is absolutely crucial for service providers to solve the challenge of a converged next-generation network and its managed architecture"

1.4 Market Trends and Challenges in Communication Technology

In the past few years, the growth in consumption of broadband services has not kept pace with falling prices for bandwidth from service providers. As a result, the service providers are transforming their existing network infrastructure into a newer form of network to generate high-margin services and lower operating cost [4].

In the meanwhile, traditional service providers are seriously threatened by the small scale service providers with value-added services and high revenue- generating services. There are two ways to overcome this worse case situation presented by small scale service providers. Firstly, transformation of existing network infrastructure into new attractive service platform is carried out to enhance the average revenue per user [4]. Secondly, a dramatic increase in operational efficiency will result into lower operating cost and increase the quality of service (QoS) for the customers. In the developing era of communication and information technology, structural change is under development. The classical telecomm networks were managed and implemented in order to transform specific data such as telephone or pure data packages [5].

Technological enhancement and market requirements altered the traditional attitude of the telecommunication market due to the high rate of competition between companies. Currently, the telecommunication industry has boomed due to the dramatic rise in broadband connection, various converged networks and fully unified IP-based networks. New challenges in telecommunication market such as Internet telephony and Mobile telephony are signs of competition for traditional telecommunication operators [5].

The network operators are making more new trends in the telecomm business in order to facilitate these coming challenges. The boundaries between fixed networks, mobile networks and data networks are merging together for the provision of a wider range of services on a single platform. The merging of these networks requires a Meta Infrastructure called core network. The new core network based on Internet Protocol (IP) is called Next Generation Network [5].

2 Next Generation Network

According to International Telecommunication Union (ITU):

1:- The network used for the provision of end-to-end voice, data and multimedia services in the presence of core network with full quality of service (QoS) capabilities is called Next Generation Network (NGN). The services provided by NGN based on Internet Protocol (IP) due to its flexibility and simply integration of new applications [5].

2:- The Next Generation Network is used for convergence of diverse connecting protocols and provision of voice, video and data services through applications and protocols. It has certain features such as packet based switching and networking with the transport layer separated from the application layer [6].

3:- A Packet-based Network used to provide telecommunication services such as multiple broadband, QoS-enabled transport technologies is

known as Next Generation Network. Unrestricted access is offered to different service providers through different users. Generalized mobility is provided through this network giving consistent services to the users [4].

2.1 Detailed Description of NGN

The term Next Generation Network (NGN) is used to support telecommunication network architecture and its technologies and services. Conventional Public Switched Telephone Network (PSTN) data, Voice Communication and Video Services are to be supported on the basis of NGN. The information carried through this network is based on packet switched form known as Internet network [7].

The information in packet forms is marked on the basis of their types such as data, voice and video and then forwarded to other networks based on quality of service (QoS) and security mechanisms. Next Generation Services like IPTV for broadcast TV, Video on Demand, Voice over IP (VoIP), and Online Gaming etc. are to be advertised based on separated transport and service layers of the Next Generation Network [4].

The Next Generation services can be modified or added through network service provider directly at the service layer without considering the transport technology.

2.2 Functional Architecture of Next Generation Network

The mentioned diagram shows the functional architecture of Next Generation Network. It describes the different functions, its services and interfaces used for interaction of functions with each other. The three different lines black, dotted black and dotted blues describe the media, control and management services provided to the functions.



Figure 5. Overview of NGN Functional Architecture Source: VTT, Technical Research Centre of Finland (2007).

Next Generation Network functions are to be divided into transport and service layers based on separated transport and services functions. Different interfaces are used for connection of different function with each other within NGN. An interface called user-tonetwork interface (UNI) is used for connection of end-users functions with each other. The other interface known as network-to-network interface (NNI) is used for connection of different networks having different entities. Lastly, the applicationnetwork interface (ANI) is used for implementation of third party applications [7].

There are different functions are described separately providing different services as follows:

2.3 Transport Functions

All components and physically separated functions within an NGN are to be connected through the use of transport layer functions. An IP protocol is responsible for transportation of different functions within the Next Generation Network. IP connectivity is to be supported to end-user equipments residing outside an NGN and different controllers and enablers within an NGN through the support of transport layer [7].

The transport layer has two separate access and core network with different functionalities. The functions in the transport layer are further divided into sub functions providing different services.

2.3.1 Access Functions

This is a sub function of transport functions in the transport layer connecting with end user functions. The functions dependant on access technology supported by the transport layer are used to manage end user access to an NGN network. The access technologies are categorised into cable access, DSL, wireless access, Ethernet technology etc [7].

2.3.2 Access Transport Functions

Access transport functions lie in the category of transport functions in transport layer. Information is to be carried or supported across the access network through the access transport functions. It deals with QoS control mechanisms such as buffer management, queuing, scheduling, packet filtering, traffic classification, marking, policing and traffic shaping having direct relation with user traffic [7].

2.3.3 Edge Functions

The Edge functions supported by transport layer are responsible for traffic processing after merging of access traffic into core network. These functions also have interaction with transport control functions through its own mechanism.

2.3.4 Core Transport Functions

The core transport functions are responsible for information transportation through the core network in the transport layer. Different parameters are used for differentiation of quality of transport through the interaction with transport control functions. It also handles user traffic directly on the basis of QoS mechanisms such as buffer management, queuing, scheduling, packet filtering, gate control and firewalls etc.

2.3.5 Network Attachment Control Functions

This function is a subcategory of transport control functions residing in the transport layer. It ensures access to Next Generation Services through the provision of registration at the access level and initialization of end-user functions. These functions are supportive for network level identification and authentication, managed IP address space of access network and authentication of access sessions. These functions support end user equipments in registering and starting to use the NGN through the central point of NGN services and application functions to the end users [7].

2.3.6 Resource and Admission Control Function

The network address and port translation control, management of differentiated services field code points are the main functionalities of admission control and gate control respectively supported by the resource and admission control function. Admission control involves authentication and authorisation based checking of user profile, operator specific rules and resource availability [7].

Transport layer functions such as packet filtering, traffic classification, bandwidth reservation and allocation functions are to be controlled through the interaction of resource and admission control function with the transport function.

2.3.7 Transport User Profile Function

This comprises of the user and control function in order to formation of single "user profile" function in the transport layer. This function may be specified and implemented in any part of Next Generation Network (NGN) as a set of co-operating database [7].

2.3.8 Gateway and Media Handling Function

Gateway functions are used for interaction between more than one network such as a ISDN/ PSTN based network and the Internet. Media handling functions are responsible for provision of services like tone signal generation, transcoding and conference call bridging [7].

2.4 Service Functions

The Service layer has two sets of functions such as application functions and service control functions

providing different services respectively. Next Generation Network services involve session-based services such as IP telephony, Video conferencing and non session-based services like video streaming and broadcasting etc. Network functionalities with existing PSTN/ISDN services are to be supported through NGN services and functions [7]. The services functions are divided into sub categories such as service and control functions, service user profile functions, application functions etc.

2.4.1 Service and Control Function

These functions involve session control function used as a registration function with the support of authorization and authentication function at the service level.

2.4.2 Application Functions

These functions are the sub functions of the service layer providing different services. Third party service providers use trusted or untrusted application functions for NGN service layer capabilities in the service layer. Application functions are needed due to the open APIs supported by Next Generation Network. The third party service providers can create enhanced services for NGN on the basis of open APIs [7].

2.5 Management Functions

These functions ensure network management by NGN operators with additional required quality, security and reliability. They are provided to each functional entity interacting with different network element management, network management and service management functional entities [8] [9].

The management functions together with charging and billing functions interact for the collection of resource utilization information. Online interactions such as prepaid services are made confirmed through collected charging and billing information.

2.5.1 End User Functions

These functions have direct relation with the service control functions as well as application functions through user-to-network interface (UNI) as shown in the above mentioned figure. Customer interface connected to a Next Generation Network cannot be limited through ITU-T specifications. All types of customer equipments range from single telephone to complex networks are to be supported by NGN. These end-user equipments are to be categorised into two such mobile or fixed [10].

3 IP Multimedia Subsystems

IP Multimedia Subsystem is a central part of the Next Generation Network having different functions and entities. Session based services provided in Next Generation Network are to be supported through the IP protocols IP Multimedia subsystem. The 3rd Generation Partnership Project was the responsible for IMS defined in both mobile networks as well as in NGN. IP Multimedia Subsystem has partly no concern with network access technology. IMS use Session Initiation Protocol as a signalling protocol used for the creation, modification and termination of the sessions [11].

3.1 IMS Architecture

IP Multimedia Subsystem architecture has different functions and entities and it is a central part between both core and access networks. Basically, these two networks are separated by 3rd Generation Partnership Project IMS definitions. More than one radio access network is to be connected to the core network in wireless network model [12].

The radio access network is responsible for the connection establishment between terminal and services in the core network. For IP transport connectivity provision between a user domain and a core transport network, an access network having multiple entities is to be used. Different access networks are distinguished on the basis of underlying technology, ownership or administrative partitioning. Core network functional entities defined by an IMS are used to provide IP transport connectivity between one or more than one access networks and core transport networks. The core network providing connectivity to service layer entities can be distinguished on the basis of underlying technology, ownership or administrative partitioning [7].

User mobility support is an important feature of IP Multimedia Subsystem. User mobility is used to ensure distinction between core and access network. In the below mentioned figure, all supported networks such as access, core and transport are to be shown. In the Next Generation Network environment, a user can move from one access network to other access network maintaining its original core network services.



Figure 6. Network Partition on the basis of IMS Source: VTT, Technical Research Centre of Finland (2007).

3.2 IMS Functional Entities

An IP Multimedia Subsystem (IMS) has multiple functional entities having different functionalities. In the below mentioned diagram, there are multiple functional entities and reference points defined by an IMS functional architecture. Each entity has its own set of functions described as follows:

3.2.1 An Application Server

All IMS service control is to be managed through an application server. The server has its direct connection with Session Control Function (S-CSCF)

or Open Services Architecture (OSA) over an ISC reference point based on third party application. All SIP messages are to be carried over an ISC interface to or from an S-CSCF. The AS is used to obtain subscriber profile information through the use of interaction with Home Subscriber Server (HSS) over sh-interface. Various telephony services such as call forwarding, number translation, conference control and online charging are to be supported through this application server [12].

3.2.2 A Breakout Gateway Control Function

S-CSCF forwarded session requests are to be carried through Breakout Gateway Control Function (BGCF) for selection of network with PSTN attachment point. Local MGCF or a peer BGCF in other network is also selected through it. Selection of BGCF in other network requires optimised routing from other visited network to the PSTN. Now, the below mentioned diagram will be described, having IMS functional entities and reference points [7].





3.2.3 Call Session Control Functions (CSCF)

Call Session Control Functions (CSCF) functions are used for managing session features such as routing and resource allocation with the support of other network entities. CSCF routes the SIP invited messages to the called terminal through resource allocation after call initiation by SIP-enabled terminal. CSCF routes SIP messages to the BGCF based on traditional PSTN phone number of the called side. Breakout Gateway Control Function (BGCF) chooses Media Gateway Control Function (MGCF) for the signalling conversion [7]. Three types of control functions such Serving CSCF, Interrogating CSCF and Proxy CSCF as follows:

S-CSCF is to be used as a registering function and establishes the relation between user ID and terminal location after accepting SIP register requests [12]. S-CSCF gets a subscriber profile with filter criteria indicating service control to the user through ASs. The S-CSCF interacts with these ASs during the SIP signalling mechanism for supporting service control.

C-CSCF monitors the Session Description Protocol (SDP) to make sure session availability within subscriber's profile boundaries during session establishment. SIP messages are to be routed through S-CSCF on the basis of originating user equipment. It uses the destination name of the terminating subscriber for getting address of an I-CSCF from a domain name server (DNS) and then forwards these requests towards the destination.

The S-CSCF forwards the SIP request to a BGCF for routing towards the destination on the confirmation of the terminating subscriber name as a PSTN address. After that, the S-CSCF forwards the SIP requests towards the P-CSCF according to the subscriber's registered location on the basis of destination endpoint. I-CSCF treats the IMS home network as an initial point of contact from the other network [12]. Stateless SIP proxy functions are to be performed by I-CSCF and SIP requests are to be sent towards user assigned S-CSCF.

P-CSCS treats IMS user terminal as an initial point of contact. It sends SIP register requests from the UE to an I-CSCF residing in a home network through the performance of a stateless SIP proxy function. UE provides a home domain name for the finding home network. All subsequent SIP messages from the UE are to be sent towards S-CSCF during the registration procedure [12].

3.2.4 Home Subscriber Server (HSS)

The Home Subscriber Server supports all IMS-level authentication keeping the IMS subscriber profiles and database. The HSS keeps a record of the currently assigned S-CSCF. The home network having more than one Home Subscriber Servers depends on the number of subscribers, equipment capacity and organization of the network.

3.2.5 Media Gateway Control Function (MGCF)

Inter working between the IMS and the PSTN is to be supported through Media Gateway Control Function (MGCF) performs translation between SIP messages and Integrated Service Digital Network User Part messages [12].

3.2.6 Media Resource Function Controller (MRFC)

Media stream resources of MRFP and media services such as transcoding and conferencing are to be controlled through the Media Resource Function Controller.

3.2.7 Subscription Locator Function

The SLF can be used in a distributed HSS system as a front end. The I-CSCF uses Subscription Locator Function to get the name of the HSS having required subscriber specific data during the registration and session setup. The SLF can be used by S-CSCF during the registration as well as by an AS in relation with the Sh interface. These functions are also used in server farm architecture of HSS environment.

4 Next Generation Network Reliability

NGN is a blend of both a circuit switched as well as a packet switched network with next generation services such as Online Gaming, IPTV, Video on Demand etc. It is not easy to predict NGN reliability in comparison to conventional PSTN network or the Internet due to the presence of both circuit and switched networks. Here, there will be a discussion of some improvements in NGN to ensure its reliability as compared to Internet or other networks.

4.1 Performance Concerns

NGN is the IP based same as the Internet technology. There are the following reasons relevant to the NGN performance and its reliability going to be discussed such as:

- Open and distributed nature
- Inherent scarcity of security mechanisms
- Complicated network architecture
- Presence of mission-critical applications
- Deployed before fully established
- Less number of expert solutions for efficient management
- Time and cost required for NGN integration and configuration

It is easy for a network provider or application developer to develop NGN applications due to its open architecture. Malicious applications such as end-user or control applications will be difficult to develop due to this issue. It is not easy to locate and eliminate the observed disturbance of a Next Generation Network with a distributed architecture. Modified PSTN functions used in packet switched networks result in the degradation of communication security. For example, modification is required in numbering scheme (E.164) used for an addressing mechanism. The new telephone number mapping scheme based on internet's domain name server system has the same problems such as distributed denial of service and DNS pollution happened in present [7].

Banking, medical systems and power station control are the types of mission-critical applications which require error-free transport, short response times and absolute security respectively. There is no surety of IP packet delivery due to packets dropped or delayed through the Internet type of transport data. The reason for packet dropped or delayed is overloaded network. Spoofing techniques such as source routing, flooding are significant problems in Next Generation Network due to its open architecture [7].

Network functionality performance is guaranteed through conventional circuit switched networks redundancy [7]. Packet switched network performance is maintained through less redundancy as compared to circuit switched network on the lower cost. Reliability and availability of next generation services will be available on the establishment of Next Generation Network. The new redundant links, latest network devices and software modules are to be used for the provision of reliability in the NGN. The new network has more complex architecture due to integration of conventional network with all IPbased network technology. The new network implementation is more time consuming and costly due to its more complex structure.

Essential control and management connections will make it possible for networks to be more secure with better performance and stability. The NGN concept will provide a direction for network provider and operator to built secure and coherent network and products. Meanwhile, it will be difficult to predict NGN's performance and reliability to reach the established PSTN used network level.

4.1.1 Enhanced Internet Quality

Next Generation Network services are provided with better technology in the performance of an IP Multimedia Subsystem as compared to the Internet. The IMS makes sure of provision of a robust multimedia system with the support of specific profiles and enhancements such as operator control, security, billing etc. IMS needs additionally vertical interfaces to provide following functions:

- Accounting, security, subscription data and service control require common interface to application servers
- Coordinated and enforced QoS
- Session-based media gating based on operator control
- Services, session and transport layers need correlated accounting and charging

The above mentioned features are responsible for the formation of an IMS structure. The Next Generation Network can be distinguished from the Internet on the basis of session control point of view. Based on all theoretical views about the NGN complex structure, results come in the more reliability and more controllable [7].

5 Motivation for NGN

The motivation for Next Generation Network is to provide a central platform through convergence of multiple networks. The aim is to bring all existing networks with different transport and control technologies into a unique, unified and multi service platform based on an Internet Protocol (IP) [5].

Growing trends of telecommunication de-regulation and rapid convergence of distributed computing and communication are the main two factors for the development of this future based network. Overall, the purpose of this new network is to cut costs, to create new income sources and provision of next generation services etc.





In the above mentioned diagram, there are three reasons of the establishment of a Next Generation Network such as Heterogeneity of telecomm infrastructure, growing competition from other sectors and falling call sales. There will be description for each reason in the development of NGN as follows:

5.1 Heterogeneity of Telecommunication Infrastructure

These days, modern telecommunication involving satellites, mobile phone networks such as GSM/GPRS, wireless LAN, WiMax and Bluetooth provide new services like Video on Demand, telephony Voice over IP, Games on Demand and Content Cashing or VOD casting etc [5].



Figure 9. Heterogeneity environment of NGN and relation with legacy network Source: Centre for

Telecommunications Access and Service (2007).

NGN has been built up on the heterogeneity concept in the presence of multiple traditional networks such as the fixed PSTN/ISDN, second Generation Mobile Networks and the Internet. In the above mentioned diagram, multiple networks with different services have converged on the single platform called core network or Next Generation Network.

The NGN infrastructure is divided into different categories such as legacy networks like 2G GSM, 2.5G GPRS, and PSTN/ISDN. Gateways such as Signal Gateway, Media Gateway, IVR, Trunking Gateway, Media Gateway, NAS, and GGSN are used for connection establishment between legacy networks and core network. The Core network is responsible for the provision of multiple services with the quality of service (OoS) in the presence of packet transport network. The transport laver separates the service and connection control implemented in a soft switch. Whereas the Next Generation Network establishes connection with the existing circuit switched network via signalling, trunking and media gateways [13].

The increasing services require their platforms which in return add complexity to the overall structure. To overcome interoperability problems and complexity due to these services, more staff and operating costs are required.

5.2 Growing Competitions from other Sectors

Different network suppliers provide services of mobile telephony, data network and fixed network individually. An interaction of various complementary elements is required for the provision of network services and products. It is compulsory to make a difference in value added level such as hardware for availability of services in the network. Development of a new, digital value-added chain is possible due to the increased use of IP-based networks.

6 Planned Targets of NGN

These days, multiple networks providing different services are converging in a unified, common platform to implement future targets and market trends. There are two main contributions of Next Generation Network made by network operators. Firstly, the optimized network will create the potential for cost saving and the other is to maintain new income resources in future [5].

6.1 Cost Reduction

The network operator makes it possible to make a sustainable infrastructure to meet the challenges of converged network environment in the presence of Next Generation Network. It keeps its interest on cost saving potential through establishment of single technology system. The single technology system will be used to cut down staffing requirements. NGN is based on a modular structure with a simple and cost effective infrastructure [5].

6.2 New Sources of Income

A unified and consistent Next Generation Network provides the source of income for established network operators to ensure next generation services. The network operators have expectations in sales opportunities of new emerging value-added services such as online gaming, video on demand, virtual reality, video conferencing and business TV in Next Generation Network [5].

7 Next Generation Network Services

A converged, unified, and data-centric network provides multiple services with different quality and cost parameters under one umbrella or core network called the Next Generation Network. Currently, the existing traditional networks are in the transition phase of transforming their infrastructure to adopt new innovative services with a better quality of service and lower cost. There are many services are linked with the existing Next Generation Network platform but some require its advanced control and management features [14].

The unified, converged Next Generation Network services are linked with access, transport and routing services. Now, the services offered by NGN re discussed as follows:

7.1 Voice Telephony

The Voice Telephony services such as Call Waiting, Call Forwarding, 3-Way Calling, Various Centrex and various AIN features are to be used by the Next Generation Network. Mostly services are implemented through NGN but it is not compulsory to duplicate each telephony service for it. NGN will concentrate on enhancing voice telephony services according to market trends and customer needs [14].

7.2 Data (Connectivity) Services

Next Generation Network provides data connectivity services used for real-time connectivity establishment between end-points with the support of value-added features such as bandwidth-on-demand, connection reliability, resilient Switched Virtual Connections, bandwidth management and call admission control etc [14].

7.3 Multimedia Services

The services used by the Next Generation Network (NGN) provide interaction between multiple parties using voice, data and video etc. It uses visual information for conversation between different customers. Collaborative computing and groupware are to done through this service of NGN.

7.4 Virtual Private Networks (VPNs)

Interlocation networking capabilities of businesses can be improved through voice VPN technique. Voice VPN provides uniform dialling capabilities to the subscribers of small private organizations [14]. Data VPN with extra security and networking features are used to provide shared IP network as a VPN.

7.5 Public Network Computing

These services are used for businesses and consumers to provide public network-based computing services. For example, generic processing and storage capabilities such as storage or maintenance of data files are provided through public network provider. Specific business applications like Enterprise Resource Planning, Time Reporting and consumer applications such as TaxCut, Kitchen Remodelling program are provided though the public network provider [14].

7.6 Unified Messaging

This service of NGN ensures the delivery of voice mail, email and fax mail through common interfaces. Users will be accessed and notified of different message types without having any means of access such as wireline or mobile phone.

7.7 Information Brokering

Consumers with providers matching are done through advertising, finding and information. For example, information can be received on the basis of prespecified criteria or personal preferences.

7.8 E-Commerce

E-Commerce is also a new service provided by Next Generation Network. It involves online transaction processing, payment information verification, security provision and possibly trading based on negotiation of goods between sellers and buyers. Home banking, home shopping, business-to-business applications like supply-chain management and knowledge management applications are also this type of service [14].

7.9 Call Centre Service and Interactive Gaming

This service enables the virtual call centre and subscriber to place a call to an appropriate agent anywhere, anytime by just clicking on the web-page. Next Generation Network offers this service to establish interactive gaming session for consumers.

8 Conclusion

This paper has clearly focused on the presence of an IP-based Next Generation Network. It provides a cost effective infrastructure for new network services providers and provides valued added services. The main part of the NGN is an IP Multimedia Subsystem (IMS) used to provide all session based services with the help of signalling protocol. IMS uses Session Initiation Protocol as signalling protocol used for the creation, modification and termination of the

sessions. The NGN and its supporting technologies are dynamic and will evolve over time. The IP based NGN uses an internet protocol as a basic transport mechanism and provides a more complex infrastructure in the presence of existing networks. The further research is still required for finding cost effective solution provided by NGN.

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MODEL OF THE ELECTROMAGNETIC LINEAR ACTUATOR FOR OPTIMIZATION PURPOSES

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KEYWORDS

Multidisciplinary modeling, electromagnetic linear actuator, optimization, genetic algorithms.

ABSTRACT

The goal is to present a more accurate model for optimization of design and of a supply control. The object is an electromagnetic linear actuator which is built of series of coils and of a ferromagnetic moving core. The coils are supplied by time series of current impulses. Even though that linear electromagnetic actuators are commonly known their applications are not wide. This is mainly because of the low energy efficiency. The efficiency is here understood as a ratio of the kinetic energy of the core at the outlet of the device to the electric supply energy delivered to the coil. The efficiency can be improved by design parameters optimization and by the accurate supply control, as well, but an adequate accuracy of the mathematical model is required for optimization process. In this paper a simulation model is presented, with a careful consideration of the hysteresis of ferromagnetic parts, of nonlinear distribution of the magnetic field and of the dimensions of all coils. The time-dependent nonuniformly distributed magnetic field is analyzed by the FEM method. The computer simulation results and experimental data of magnetic flux density are compared. Special sensors of the Colossal Magneto-Resistance (CMR) effect have been used for verification of the simulation results (Balevicius et al. 2005, Schneider et al. 2007). The Multi-Attribute optimization has been completed and the Pareto set is defined, by evolutionary optimization methods.

INTRODUCTION

In many industrial processes like riveting, hammering, marking, making holes in hard or crisp materials, connecting of metal sheet using a cold-forming process, etc. linear actuators with the high velocity of displacement of the moving part are necessary. If the velocity is of a prime importance, electromechanical actuators may be useful. The main advantages of the electromagnetic linear actuators are the simple design

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) structure, the fast response for the input signal, a possibility to achieve a high linear acceleration and a low cost of the maintenance. Moreover, a linear motion is a natural output, so there is no need of any mechanical transmission. On the other hand, the main drawbacks are: a low energy efficiency and a need of the great power current impulse source (Howe 2000, Seog-Whan et al. 1996).

The linear mathematical model of electromagnetic actuator is sufficient in many considerations, but not if a more accurate calculations are needed (Tarnowski 2004). Such model can be used for investigation of the influence of some part of the object and then an optimization of the object is possible. For that reason, the number of assumptions and simplifications should be omitted.

OBJECT OF INVESTIGATION

The general design of the electromagnetic linear actuator is presented on Figure 1. It is built of a series of coils and of a ferromagnetic or magnetic moving core. The coils are supplied by series of current impulses. Here only a single coil system is discussed.



Figure 1: General design of the electromagnetic linear actuator

THEORY - MATHEMATICAL MODEL

The magnetic coil energy and the electric energy are coupled, and the interchange depends also on the position of the core. What more, eddy currents are induced in the core. A distribution of the magnetic field is not uniform neither in the air gap nor in the ferromagnetic parts of the devices so it must be modeled as a continuous in space. If the core velocity is not high, the air pressure resistance may be omitted. Also electrical properties may be accepted as discrete in space, as the current changes in coils are comparatively slow. As the motion process of the core is short, the temperature increase is small and the process may be assumed as an isotermic and all material parameters to be constant, unless the process is repetitive with the same core. To summarize, there are many nonlinear phenomena, and they are strongly coupled.

Electromagnetic filed

The hysteresis of electromagnetic parts and the nonuniform distribution of the magnetic filed should be included (see Figure 2). The non-analytic relation between the magnetic field strength H and the magnetic flux density B can be described as a table with series values and then introduced into computer model (ComsolMultiphysic's User's Guide 2003).



Figure 2: Hysteresis of the ferromagnetic part

Distribution of the electromagnetic field of the linear actuator can be described by the Maxwell equation:

$$\sigma \frac{\partial A}{\partial t} + \nabla \times (\frac{1}{\mu_0 \mu_r} \nabla \times A) - \sigma \nu \times (\nabla \times A) = j_{ext.}$$
(1)

where:

 σ – electric conductivity; μ – permeability; $j_{ext.}$ – current density due to an external source; A – vector potential; and the magnetic flux density is given by:

$$B = \nabla x A \tag{2}$$

When we write this equation in the cylindrical coordinates, the symmetry assumptions imply that both the external current density j_{ext} and the vector potential

A have only an angular component, and the derivative with respect to the angle vanishes. Rewriting the rotation operator in cylindrical coordinates, we obtain Maxwell's equation for the angular component ψ . It can be defined as a new dependent variable:

$$u = A_{\Psi} / r \tag{3}$$

Writing $\nabla = (\partial_r, \partial_z)$, we obtain the form of the Maxwell equation which has been used in simulation:

$$\sigma r \frac{\partial u}{\partial t} - \nabla \times \left(\frac{1}{\mu_0 \mu_r} \nabla \times u\right) - \frac{\partial}{\partial r} \left(\frac{2}{\mu_0 \mu_r} u\right) + \sigma(r v \nabla u + 2 v u) = j_{ext,w}$$
(4)

Electrical sub-system

One way to define the current source is to specify a distributed current density in the right-hand side of the equation 4. The current I may be calculated as an integral of the current density:

$$\int_{S} \rho_{j} ds = j \tag{5}$$

Current density ρ_j in a coil is limited by the heat losses and capabilities of power supply:

$$\rho_j \le \frac{j_{\max}}{\frac{\pi l^2}{4}} \left[\frac{A}{m^2}\right] \tag{6}$$

where: d – is a diameter of copper windings of coil. The number of winding-turns is a function of dimension of coil and the fill factor:

$$a \cdot b \cdot \rho \cdot 0,7 = j_{\max} \cdot z \tag{7}$$

where: a, b – are dimensions of coil (see Figure 1).

Mechanical sub-system

For computing the total electromagnetic force the equation presented below has been used:

$$ma = \int_{\Omega_1} \rho \frac{d^2 r}{dt^2} dV = F \tag{8}$$

The total force is computed as a boundary integral of the stress tensor in vacuum on the outside sub-space of the solid. The contribution from the air pressure gradient has been neglected. The electromagnetic force implemented in Matlab program is used for computing the displacement value.



Figure 3: Exchange of data between programs

The mechanical equations have been implemented in the Matlab program and the Maxwell equations have been used by ComsolMultiphysic's. Two programs are working together respectively. In the Figure 3 an interchange of data between the two programs is shown. The simulation results are presented as a sequence of series points in the Figure 7, 9 and 11.

SIMULATION AND EXPERIMENTAL RESULT

The goal of experiments was to check a possibility to measure the electromagnetic flux density B inside the coil and to verify of the simulation model. In the Figure 4 the view of the model implemented in the FEM program is shown. In the Figure 6-11 magnetic flux density is presented as a function of time for the better analysis of the simulation result.



Figure 4: Magnetic flux density simulated in the FEM model

Experiments have been conducted for three cases:

- coil without ferromagnetic core;
- coil with fixed ferromagnetic core;
- coil with moving ferromagnetic core.

Special sensors of the Colossal Magneto-Resistance (CMR) effect have been used for verification of the simulation results.¹ Figure 5 shows a schematic diagram of the experimental set-up and measurement equipment.



Figure 5: Schematic diagram of the experiment and measurement equipment (Balevicius et al. 2005)

The magnetic field generator (with the main components: capacitors, thyristors and coil) is triggered by a single pulse produced by a function generator. After ignition the thyristor connects the capacitor to the coil. The trigger signal also triggered the oscilloscope, which is used for visualization of the signal measurement by CMR-sensors. The sensors were placed inside the coil in space between the inner windings of the coil and moving ferromagnetic core. For data storage, the oscilloscope output was connected to a personal computer (PC).



Figure 6: The measurement position of the CMR sensors with reference to the inner coil surface

¹ The experiments were performed in Semiconductor Physics Institute, Vilnius, Lithuania.



Figure 7: Comparison between experimental and simulation results for the coil without a ferromagnetic core, measured by three sensors (see text)

Pulsed magnetic fields were generated by a multiple winding coil with 25 windings in each of 4 layers, outer diameter of 32 mm, length of 60 mm, and inner diameter 14.4 mm. The resistance of the coil was $R_0 = 0.2 \text{ m}\Omega$ and the inductance $L_0 = 40 \text{ nH}$. The pulse power generator included a capacity of 2240 μ F. The sensors were situated in center of the coil in distance 5 mm from each other. The experimental results are presented as the three color lines in the Figure 7. The magnetic flux density was measured as a function of time and achieves value of about 1.4 T. The simulation results are presented as small triangles in the Figure 7. The simulation and experimental results are very similar.



Figure 8: Sensors system for the magnetic field with fixed ferromagnetic core

Another experiment was to simulate magnetic flux density changes as a function of different current in time with fixed ferromagnetic core. The sensor number 1 was situated in closed distance to the ferromagnetic core. The sensor value is smaller than for the sensor number 3 situated out of the core. This is because nonlinear distribution of magnetic field disturbed by ferromagnetic core inside the coil. Some of the result simulation was presented as a triangle (for the place where sensor number 3 is situated) and circle points (for the place where sensor number 1 is situated) in function of time and current value.



Figure 9: Comparison between experimental and simulation results for the coil with fixed ferromagnetic core, measurement by two sensors (see text)



Figure 10: Comparison between experimental and simulation result for coil with moving ferromagnetic core measurement by three sensors (see text)

The next verification of the simulation model was to measure magnetic flux density as a function of moving ferromagnetic core and as a function of different current in time. It can be seen in the Figure 11 the electromagnetic flux density is cumulated in the ferromagnetic core when the core is moving closed the sensors. The current changes are shown in the red color. The core is moving near the sensors in sequence: the sensor number 3, the sensor number 2 and the sensor number 1. The triangle points in the Figure 11 are the simulation results respectively to the place of the simulation points. The simulation points are the same as the place of CMR sensors.



Figure 11: Comparison between experimental and simulation result for coil with moving ferromagnetic core measurement by three sensors (see text)

OPTIMIZATION PROCESS

Having completed a verification and validation of the simulation model an optimization of the actuator design may be considered (Fischer et al. 2003, Tarnowski 2004). The poly-optimization problem which is shown below is to be a proof that the presented simulation model is generally capable for optimization.

The goal of the system is to accelerate the ferromagnetic moving core to achieve a demanded kinetic energy, with restriction to the dimension and the total mass of the device. The main functional criterion is the power efficiency - here understood as a ratio of the kinetic energy of the core at the outlet of device to the electric supply energy delivered to the coil. An important parameter is the outlet velocity of the ferromagnetic moving core: if one demand a high speed, also the current in the coil must quickly increase and after a very short period of time decrease to zero. To achieve it by a constant voltage, a small inductance is necessary. Thus we decide to adopt the coil inductance as another optimality criterion. If the electrical power supply subsystem is unable to deliver such a short impulse of current, the dimensions (and the mass) of the ferromagnetic moving core should be changed and optimization process should be resumed.

The adopted decision variables are: dimension of the coil (a, b - see Figure 1), dimension of the ferromagnetic moving core (d, r - see Figure 1). The inner radius of coil is almost equal to the outer radius of ferromagnetic core.

In the past, the optimization process was conducted by full decision space survey approach (Piskur and Tarnowski 2007). But this technique is not very efficient naturally. Gradient methods seems to be not very efficient due to the fact, that single goal function computing takes not less than 20 seconds and what more we have had no initial knowledge about the shape of the goal function (a monotony and local minima).

To find the optimal solution(s) we adopt the genetic algorithms techniques. It is important how many

decisions variables are used, how many iteration should be declared and how numerous population should be adopted.

The number of genes and iteration are limited by the computer power. What more the genetic algorithms enable to determine the minimum value of force and the maximal value of the coil inductance as the penalty function in the fitness function. In the Figure 12 the example of evaluation function is shown. On the vertical axis the inductance of the coil value is presented and on the horizontal axis the electromagnetic force is presented. As the optimization process is searching for the minimal value of the function the electromagnetic force is set as negative amount.



Figure 12: Example of the Pareto optimal solution.

METHODOLOGY OUTLINE

To complete an adequate mathematical model the following actions are recommended:

- 1. Definition and specification of the object and its environment. On the basis of designation of the model, determination its accuracy and scope of validity.
- 2. Identification of all processes and relations in the object.
- 3. For each phenomenon define assumptions and simplifications. Taking a decision whether the phenomenon is space distributed or discrete. If distributed, assuming continuity, symmetry and number of space dimensions (1D, 2D or 3D)
- 4. Definition of mathematical relations.
- 5. Decision on how to solve the model. As the rule, it comprises nonlinear partial or ordinary equations, so computer programme is necessary. A commercial package would be the best choice, but in the case of many various energy streams involved (eg. Multiphisics case), probably one does not find any commercial code and one must device a special programme.
- 6. Verification the code; validation the model.

CONCLUDING REMARKS

Mathematical modeling of dynamic transient processes for computer simulation purposes in some objects requires that a few various energy streams must be considered (the Multiphysics case). Also in many cases the energy density field is non-uniform in the 3D space, so the partial differential equations must be applied, and they are non-linear if a better accuracy is expected. As a rule, they have no analytic solutions, and the finite element paradigm is to be used.

For the object under consideration a multidisciplinary model must combine the finite element analysis with other computational engineering tools and applications such as the control system design, signal processing and dynamic simulations.

Because of the model symmetry and the long simulation computation time only half of the electromagnetic device has been to take under consideration. In this model a few physical phenomena is solved simultaneously. It can be useful to observe much output information in specific points of the device as a function of input construction data.

An adequate accuracy of the model is required for optimization process. In the future investigations the multidisciplinary model will be used for the control algorithm optimization process.

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On the Design of the DISO Controllers for a Neuro-Fuzzy Vector Control. The training data acquisition.

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KEYWORDS

Neuro-fuzzy, Vector Control, Electrical Drives.

ABSTRACT

The paper deals with the synthesis of some neuro-fuzzy speed and current controllers for a vector control based structure associated with an asynchronous motor and an inverter. Many operating conditions for the system are taken into account, like speed reference profile (including some special ones for a smooth motion in a transportation system), quadrants, load torque etc. The final goal is to substitute all the standard controllers with neuro-fuzzy variants, able to ensure a high robustness so that the influences of the motor parameters, load torque, sampling period and operating conditions could be minimized and good global performance could be achieved. The paper intends to reveal some details not directly visible applying an automatic neural network training procedure for the generating the fuzzy controllers. However, these details could improve the solutions. The results are compared with those from the initial / reference system.

INTRODUCTION

The fuzzy logic controllers (FLC) and the artificial neural networks (ANN) represent new tools in the analyze and the design of the electrical drives. Many papers deal with the applications of one or more of the artificial intelligence tools in the field of electrical drives with induction motor (IM) and the associated power electronics (Bose et al. 1997, Minth 1997). Some books and papers are oriented especially on applications (Bose et al.1997), (Godjevac 1997) - the last one being dedicated to the robotics, drives / motion control. It seems that using FLC for the control of asynchronous motors is not a very new idea. But the variety of approaches is very big. (Abad et al. 2005) proposes a fuzzy controller for the speed control for an IM with constant flux. Some researches concern the modeling / identification of the system (complex, non-linear) by neural networks or using ANN for the asynchronous motor speed estimation in order to improve existing control strategies. Others try to find solutions by neurofuzzy models for detecting faults in the IM. Fewer papers are allowed for a vector control (VC) including FLC. However, some books and papers give more or less detailed guidelines for the IM and VC: (Caron and Hautier 1995, Roye 1997, Canudas 2000, Huy 2002).

Although stated as a high quality strategy for the IM control (one of the best, anyway – (Leonhard 1997)), there are some important drawbacks related to the parameters sensitivity. The effort paid to overcome this problem is very important. In that meaning, (Rehman 2005) is a proof for how complex is any method trying to suppress the stator resistance sensitivity.

Tuning for an optimized VC by on-line procedures is a very challenging task, involving several difficulties and complex methods - (Lin and Yang 2003). (Lin and Hsu 2002) gives an ANN - based solution for the adaptive control for an induction servodrive. An early paper (Buhl and Lorenz 1991) proposes an ANN solution for the digital current regulation of inverter drives. (Hautier et al. 2004) makes a study for a fuzzy supervisor for an optimal VC in term of the best flux estimation. In (Shewy et al. 2005), beside a modeling of induction motor using feed-forward neural networks (usable mainly in speed-sensorless estimation), a brief list of research directions and results is inserted. One of the most representative references in the field, especially in terms of a wide range of results using the Artificial Neural Network (ANN) for the induction motor control, is (Vas 1999).

The author proved by several previous results – (Mihai and Constantinescu 1999), (Mihai and Vasile 2007) that a well tuned fuzzy loop is able to compete and outrun the standard digital algorithms for DC servodrive and for the IM systems lead by VC strategy. In some applications, an off-line pre-processing associated with FLC is justified by a high quality of the results; however, the top advantage of the fuzzy logic - its simplicity - is diminished. Another way is to use only input-output data. Then, a FLC design method is based on the training of an ANN. After some promising results in substituting the conventional speed controller in a VC structure for the IM, the aim of the paper is to analyze now the abilities of the VC - FLC - ANN control part to offer good or high quality solutions for a high demanding application in terms of torque and current ripple, fast transient response, smooth motion, limitation of the over current. The results are compared with those associated with standard control algorithms. Not only that this kind of classical controllers (and their loops) are not robust, but their tuning (although stated as well settled) seems to be very difficult in complex conditions. (Koczowski et al. 2005) concerns a PID control robustness and shows some recent efforts, ideas and methods, revealing how difficult such a task is. Obtaining a large amount of training data in various

operating conditions from an experimental platform could mean a very hard work, a lot of wasted energy and time. Besides, some modifications for motor or system parameters are not possible in a controllable manner without a big cost. It is much more convenient to use a computer model and simulations. For having appropriate input-output data, the first step is to make a good tuning of the initial VC system.

Several induction motors, in the power range 2-37 kW, were considered for designing the fuzzy logic controller for the velocity loop and the current loops of a vector control structure using the IN-OUT training data acquired from a well-tuned standard VC system.

By the ANFIS method (Jang 1993), the appropriate speed and current neuro-fuzzy controllers (NFC) are generated. Then, a tuning for such controllers is performed for the local and global performance criterions improvement. In the next sections, are considered only the standard notations, SI units, time in seconds and the most of the results concern a 7.5 kW and 1456 rev/min motor.

THE INITIAL MODEL FOR TRAINING THE NEURAL NETWORKS.

The fig. 1 gives the image of the vector controlled system) with a PI speed controller and 3 hysteresis current controller, the evolution of the main variables and of some samples of the In-Out training data for the speed and current NFCs. For the tuning of the initial FOC structure, the velocity loop is simplified in an equivalent form as in the fig. 2. From the motion equation, with a PI controller ($k_{p\omega}$ and $T_{i\omega}$ as tuning parameters), the next relations are derived:

$$\Omega = \frac{1}{J_{s+f}} \times (T - T_{load})$$
(1)

$$\Omega = \frac{1}{Js+f} \times \left(k_{p\omega} + \frac{1}{sT_{i\omega}} \right) \times (\Omega^* - \Omega) - \frac{1}{Js+f} \times T_L \quad (2)$$

After some calculus, identifying the results with the standard form, the next algebraic system is obtained:

$$G(s) = \frac{1}{1 + \frac{2\xi}{\omega_n} s + \frac{s^2}{\omega_n^2}} \begin{cases} J \times T_{i\omega} = \frac{1}{\omega_n^2} \\ \frac{2\xi}{\omega_n^2} = (k_{p\omega} + f) \times T_{i\omega} \end{cases}$$
(3)

From $\xi \leftrightarrow \omega_n t_{resp}$ (t_{resp} is the response speed time of the system) – (Buche 2001) is considered an unit damping factor, so $\omega_n t_{resp 5\%} \approx 4.75$ gives the tuning parameters:

$$\begin{cases} k_{p\omega} = J \times \frac{9.5}{t_{resp}} - f \\ T_{i\omega} = \frac{1}{J} \times \left(\frac{t_{resp}}{4.75}\right)^2 \end{cases}$$
(4)

As for the tuning of the hysteresis current controller, the only parameter (Δ) has influence mainly on the current (and electromagnetic torque) ripple; so, at this point the

tuning is simple, according to a limit for this ripple and the upper commutation frequency supported by the devices inside the inverter.

For this initial model, the next possible scenarios and elements must be considered in order to deliver more or less better training data and for the NFC synthesis:

- a. The strategy for the NFC synthesis:
- first, the inner (current) controller, with the classical PI controller for the speed loop;
- first, the external (speed) controller, keeping the hysteresis current controller;
- with an unique training data set taken from the initial model, the synthesis of the NFCs being made for both of the loops;
- SISO or DISO NFCs.
- unique or adapted to each phase current NFC;
- b. Optimization of the training data set, by:
- the sampling rate for the training data (test have been made from 10 us, that meaning n x 100,000 data pairs);
- the most relevant conditions for the operating regime (with a single operating quadrant or with a reversible speed profile, maximum reference speed, load torque as type and values);
- c. The training program:
- the number of the fuzzy sets for each variable;
- the epoch number (from 20 to 30000);

- different kind of inference methods, fuzzy operators etc.

d. Post training tuning of the neuro-fuzzy controllers. By the author experience, the most suitable actions concern the redistribution of the fuzzy set so that:

- the too big surface control slopes must be avoided (the same big slopes in the input n-f controller bring bad values in their output correspondences see the lack of a SISO training instead the consideration of the error variation as a second entry for the FLC).
- the angular points must be avoided;
- the IN/OUT variables scale of the NFCs must be inner in relation with the training scale of the same variables
 some saturation blocks could be added if necessary;
- the steady-state regime from the training data must be found as input-output values in the surface control of the NFCs;

A DIRECT AND SIMPLE APPROACH

Joining the best (tuned) SISO NFCs - for the speed loop and for the current loops, the results were far from the expectations, although the training conditions for the system were the same for both synthesis. The fig. 3 presents the results for a control structure with NFCs (one for the speed, three identical for the current). Although the general behavior is acceptable (fig. 3a), some drawbacks related with the steady-state regime (speed error) and the local dynamic (fig. 3b), as well as a certain sensitivity to the speed reference values field, pushed the study toward some new ways. Some efforts paid to improve the behavior (concerning several from the above mentioned aspects) gave results (somehow better) not very encouraging. The fig. 4 could preview such a disappointment and makes difference between the training conditions. This kind of image is helpful



Figures 1: The initial system, its variables and the training IN-OUT data for the speed and current controllers.



Figures 2: For the speed controller tuning.



Figures 3b: Details for the integral neuro-fuzzy control by SISO units for speed and current.



Figures 3a: The macroscopic variables for an integral neuro-fuzzy control by SISO speed and current units.

only for the speed loop. The training of a current NFC able to deliver firing pulses for the inverter has no more this benefit because the high rate commutations - fig. 5. The merit of such approach is that it proves the possibility to operate with all loops controlled by NF units.

THE DISO APPROACH

The consideration of the error variation $\Delta \epsilon_{\omega}$ for the speed loop allows a better control of the system, the derivative of the speed being the acceleration – an essential variable for the dynamic. The monitoring of the acceleration has benefits also in control of the kinematics for the applications with reduced mechanical shocks. The data amount increases, being involved 3 training vector for each controller. The training trajectory of the neural network (NN) improves a lot, as it can be seen in fig. 6. Although this kind of result (a) could certify the quality of the training data, the direct macroscopic results are not at all good (b-d) The next actions were tested in order to improve the behavior of the system with the same NFC:

the discrete filters (z^{-1}) are suppressed for both channels : ε_{ω} and $\Delta \varepsilon_{\omega}$. The speed ripple decreases a lot, however, the steady - state error is unacceptable



Figures. 4: The trajectories for training and NN output of a SISO speed NFC for different conditions: 1 direction / 13334 data pair and 2 directions / 250001 data pairs.



Figures 5: The trajectory for training and NN output of a SISO current NFC.

(fig. 6.c) and the output of the NFC is beyond of the training range (fig. 6d) - the output of the controller reaches 18×10^5 !.

- the output of the speed NFC is saturated in the range of the initial training data. The results are much better.
 Some important oscillations of the electromagnetic torque still persist, because of the commutations of the fuzzy rules and the operation in the neighbor of the saturation levels.
- $\Delta \epsilon_{\omega}$ is computed with $T_{s \text{ model}} \ll T_{acq \text{ training data}}$ (by 3 orders of magnitude); the results have the same aspect.



Figures 6: A good training data set and, however, some bad generated results with the speed NFC.

In order to obtain better results, the acquisition procedures for the training data could be still improved (analyzing the training state-space trajectories), as follows:

- a faster sampling (a sample period of 100μ s, that meaning 130,000 n-tuples data: 2 for Input and 1 for Output), with the same rate for the discrete filters in the model;
- better operating conditions (longer cycle, other load);
- a limitation of the upper values for the first values of $\Delta \varepsilon_{\omega}$ the speed error variation, according to:

$$\Delta \varepsilon_{\omega} \max_{\max} \approx \frac{\frac{d\omega}{dt}}{\frac{t_{start}}{T_{sampl}}}$$
(5)

The figure 7 reveals by different 2D projections the accuracy of the training process in these conditions, as well as the 3D picture of the states-space trajectory.

According to a "fuzzy vision" for the behavior of the system, the variables In-Out of the speed NFC should have smooth variations, as affect of the fuzzy sets overlap, of several fired fuzzy rules aggregation and the action of the defuzzification. A comparison between the fig. 8 and 9 (for the standard system used in the training process and the system with a speed NFC) does not confirm this expectation. More, it seems that the "well temperate" behavior still existing for the SISO speed NFC is lost - see also the fig. 1. In fact, the high rate commutations of both In-Out variables of the speed NFC are normal for the DISO variant, as the direct effect of the derivative of the first input: $\Delta \varepsilon_{\omega}$. This second entry involves a supplementary sampling and its rate is related with the magnitude of the training data collection. A smaller sampling period for $\Delta \varepsilon_{\omega}$ leads to a bigger data set, hence consequences in the computation time. There are 2 main factors that influence this constraint: the training epoch number and the magnitude of the training data. In order to avoid the over-oscillations in the future In-Out variables for the speed NFC, different sampling rates were used :

- a small T_{s1} for generate $\Delta\,\epsilon_{\omega},$ close to the integration step of the model:

$$\Delta \varepsilon_{\omega k} = \varepsilon_{\omega}(k \cdot T_{s1}) - \varepsilon_{\omega}((k-1) \cdot T_{s1})) \qquad (6)$$

- a convenient $T_{s2} \mbox{ for a resonable training data amount}$:

$$T_{s2} \ge \frac{t \text{ regime}}{N \text{ max adm DATA} - 1 \text{ variable}}$$
 (7)

CONCLUSIONS

The fuzzy control brings several well-known advantages for the control of electrical drives systems. The attempt to combine a successful control strategy like the vector control with the benefit of one or more tools from the intelligence control field (fuzzy logic, neural networks) is entirely justified. The first and simple approach with a SISO structure for the controllers (speed and current loops) have proved the ability of a single neuro-fuzzzy controller at a time to obtain good performance and robustness. In order to improve this initial results, the author raised several ideas and made many test by modeling and simulation for extending the qualities of the neuro-fuzzy technique to a system having only such kind of controllers. It was proved that an important benefit is an extended robustness for very different operating cycle. The only way for obtaining good solutions is to design DISO NFCs. It could seem only another quantitative approach, but the design changes dramatically. Several aspects drive to many design details, although there is a powerful and easy to use method (and program) for generating the fuzzy controller by training the associated neural networks. The main concern outlined in the paper is the training data preparing. The results confirm that the suggested solution exists but every little improvement of the results implies a lot of subtle details and a lot of work. The fuzzy control solutions are simple and easy to obtain only for medium-to-good results.







Figures 8: The data training set: the speed error, its variation and the saturated output for the initial speed controller.



Figures 9: The In-Out variables for the speed NFC.

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On the Design of the DISO Controllers for a Neuro-Fuzzy Vector Control. The training data processing and some results.

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KEYWORDS

Neuro-fuzzy Controller, Vector Control, Electrical Drives.

After some good previous results with neuro-fuzzy controllers SISO type for the speed or for the current loops in a vector control system, now the design is orientated to the DISO units. Also, the coexistence of both controllers type as neuro-fuzzy units are considered: the speed controller - with a slow bias and the current - with a high commutation rate for driving directly the inverter. The aim is also to provide a performing and integral intelligent-based solution for applications were the mechanical shock must be controlled (such as trams-trains, personal elevators). The design of such controllers is focused on three aspects: the conditions of a good data acquisition for training by simulation of a well tuned standard system, the data pre-processing for the training of the neural networks and the tuning of the synthesized controllers. The ANFIS methods is used for generating Sugeno fuzzy controllers. Different design details and tuning procedures are taken into account. The paper is continuing a previous work.

INTRODUCTION

Neural networks and fuzzy systems are different approaches to introducing humanlike reasoning to knowledge-based intelligent systems. The integration of fuzzy logic and neural networks seems natural and full of benefits (Kasabov, 1998). Artificial Neural Network (ANN) learns from scratch by adjusting the interconnections between layers. Fuzzy Inference System (FIS) is a computing framework based on the concept of fuzzy set theory, fuzzy if-then rules, and fuzzy reasoning. Integrating ANN and FIS have attracted the growing interest of researchers due to the growing need of adaptive intelligent systems to meet the real world requirements. (Nauk, 1995) proposes a taxonomy to describe different combinations of neural networks and fuzzy systems by Fuzzy Neural Networks, Concurrent Neuro - Fuzzy Models, Cooperative Neuro -Fuzzy Models, Hybrid Neuro - Fuzzy Models. An example for the last architecture is ANFIS (Adaptive-Network-Based Fuzzy Inference System) - (Jang, 1993), (Jantzen, 1998). The first applications of fuzzy neural networks to consumer products appeared on the Japanese and Korean market in 1991. Some examples include (Fuller, 1995): air conditioners, electric carpets, electric fans, electric thermo-pots, desk-type electric heaters, forced-flue kerosene fan heaters, kerosene fan heaters, microwave ovens, refrigerators, rice cookers, vacuum cleaner, washing machines, clothes dryers, photocopying machines, and word processors. (Vieiraa, 2004) provides a comparison of artificial neural networks and neuro-fuzzy systems applied for modeling and controlling a real system. Most of studies were made in the field of the modeling / identification / estimation / fault diagnosis for the mentioned system – (Woei, 2005). Fewer papers are allowed for a VC strategy combined with fuzzy or neuro-fuzzy controller, and only some samples concern the current loop.

For designing neuro-fuzzy controllers (NFC), an initial standard vector control structure (rotor flux variant) was considered – (Doumbia, 1997). In some previous works - (Mihai 2006), (Mihai 2007), the author performed the synthesis of SISO neuro-fuzzy (N-F) controllers that could replace the classical controllers (PI and hysteresis type for speed, respectively for current) with several benefits. Unlike other studies and solutions that implement a Mamdani controller, it is about Sugeno type controllers generated by the ANFIS (Jang, 1993) program. But the author found that the designer must be advised on several aspect concerning the best operating conditions of the system for data acquisition, the training data collection preparing and the results tuning. Continuing the paper (Mihai, 2009), several designing details for these aspects are followed both for the speed and current NFCs, in the DISO variant (considering the error variation of the variables). The results are selected from a wide range of operating conditions and induction motors taken into account (in the power range 2-37 kW, having as target application the transportation systems with low mechanical shock).

THE TRAINING DATA PROCESSING

The study carried (Mihai, 2009) has revealed that the expected (from the cycle type) non-monotonical evolution of the speed is completed by more or less powerful ringing phenomena that could have several explanations. It is unavoidable a commutations between the generated fuzzy rules (sets) as well as the commutations effect. However, every effort paid in order to reduce such oscillation should improve the overall behavior of the system. And the next (natural) idea is to tray for a good (declared) data training set, some additional processing like:

a. the reduction of the samples for increasing the speed of the training procedure (for a set of $3 \times 110,000$ data

and a standard 2 GHz PC, this duration can reach many hours..);

b. a filtering of the samples, so that some discrete noises could be eliminated.

For the first step, a program was made for selecting from a N component vector V another one V_{s} , taking only the mth samples; the new vector has N_m components, as follows:

$$V_{s}(i) = V(m \cdot i - m - 1);$$

$$i = 1...N_{m} = \left[\frac{N}{m} - \varepsilon\right] + 1; \quad \varepsilon < \frac{1}{m}$$
(1)

A comparison image of the initial training data (speed loop, 110,000 sets) and the selected ones (m=5) is given by the fig. 1, both for the ε_{ω} (left) and $\Delta \varepsilon_{\omega}$ (right). Some

small differences are visible only for $\Delta \varepsilon_{\omega}$ For a bigger m (like 10), the samples of $\Delta \varepsilon_{\omega}$ become spaced out in an obvious manner. As for the second action (the data filtering), it has a bigger role for $\Delta \varepsilon_{\omega}$, where the high rate commutations could be in a direct relation with the control ringing. The question is if the filtering does not modify the useful data substance. Because the second NFC speed controller input was added as a supplementary one in order to improve the training process, what is important is the bias of this variable and not the high rate commutations and the local big slopes. In this meaning, the filtering could be useful, indeed. The fig. 2 b and c present the filtered results using a Savitzky-Golay (polynomial) FIR smoothing filter (filter 1); the other filter (denoted 2) is a fist



Figures 2: Zoomed images of $\Delta \epsilon_{\omega}$ and the effects of a single or multiple filter.

order one. Both filters have been tuned by several tests. The aspect of the training data in these conditions (after a selection procedure and a double filtering) is given by the fig. 2d. The fig. 3 certifies a good quality of the new training data set by the similarity between the trajectory of the initial system and the trajectory associated with the data generated for the speed NFC. A direct comparison between the control variable from the initial PI speed controller and the fuzzy controller delivered by training the neural network is presented by the fig. 4.

Now, joining the experience for the previous stage, a good (better) global behavior of the system with the speed NFC is expected. The fig. 5 brings the characteristic elements (fuzzy sets, graphical correlations between the variables) for a tuned speed NFC in the next conditions:

- 1 operation quadrant;

- selected and double filtered training data;

- saturation of the output for the speed controller;

- 7 fuzzy sets, 100 training epochs, max-prod-wtaver operators for the Sugeno NF controller;

A supplementary tuning of the generated fuzzy controller was made in order to reduce some spikes of the electromagnetic torque (although with minor effects on the final speed evolution). This tuning is based on the supposition that this phenomenon could be related with (generated by) some big slopes in the inputs of the FIS controller. Such zones are identified in the projection speed error - output and the fuzzy sets are slightly modified following the effect on the slope attenuation. The fuzzy sets for the speed error variation have an unusual form but the dependence output $(\Delta \varepsilon_{\omega})$ became, obviously, a smooth one.

A global results for the system with the new speed NFC is shown by the fig. 6a and the quality of the controller is certified by the fig. 6b, where a different (much shorter than in the training step) speed cycle was imposed.

The same speed NFC is tested for different operation conditions (simultaneously applied) than those from the training step:

- a step speed input;
- a much higher steady-state speed value;
- an inertia bigger with 50 %;
- the motor resistance bigger with 25 % (like for a heating effect);
- a random variation of the load torque around the training values.

The results from the fig. 7b could give, again, an excellent mark for the NF controller, compared with the initial PI speed controller (fig. 7.a) - considering that the training of the NF solution was made in very different



Figures 3: The state-space trajectories for the selected and filtered data and for the generated speed NFC.





Figures 5: The fuzzy description of the speed controller.

operating conditions. Other test was made with no load torque (only a friction component, depending on speed); the results had the same quality.

3. THE SYNTHESIS OF THE CURRENT NFC.

The substitution of the standard current controllers (hysteretic type) that deliver directly the firing pulses to the inverter by NFC units is very challenging by several reasons:

- the high rate commutations (with sudden rise and fall edges) that could be not quite appropriate for the "continuous" approach specific to the fuzzy logic;
- the training data does not obey a bias that could characterize the IN-OUT functional relation;
- the sampling is much higher than for the current.

However, the author has succeeded to obtain a viable current SISO NFC in a system having a classical speed controller (Mihai, 2007), designing a special block for the training data acquisition (and, later, for the pulse generation by the NFC). The fig, 8 gives the image of such a block for 3 DISO current NFC, one for each phase. The aim of the study at this level is to answer and overcome the next problems:

- which is the image of the current error variation and how important is to manage this variable;
- which are the best operation conditions for the data training sampling: initial tuning of the current loops, operating quadrant, speed reference type etc;

- if it is possible to avoid some big spikes (commutations) on the power part, due, mainly, to the extrapolation type computations that the training of the NN brings especially in the edge regions of the variables range;
- if the reduction of these spikes is a matter of the training step or is related with a post-tuning procedure;
- which is the best sampling rate for the training data;
- how long must be the training time interval?
- if a values selection and filtering is useful for the current too;

According to the simulations of the initial model (and the one having a speed NFC) gives a PWM commutation frequency under 25 kHz. Then, a 30 µs sampling rate seems good. A shorter (than for the speed controller synthesis) cycle of 5 sec leads to 166,000 samples for each phase. The acquisition block from fig. 8 stores both saturated and non-saturated variables -(Mihai, 2007). The fig. 9 presents the samples c_k , c_{k-1} , Δc_k non-saturated (the upper windows) and the same saturated variables (lower windows), justifying the necessity of the saturation procedure. There is, always, a high first values zone that makes the controller insensible to the common operating values during the most part of the regime. As a result, the obtained fuzzy controller is not able to realize a (suitable) commutation. That is why an additional bloc (D-sat) for an anti-windup behavior was added in the acquisition



Figures 7: A comparison between standard and NF speed controller.

model, inserted also, later, in front of the final fuzzy controller (Mihai, 2007). Now, the FLC output is variable but not in a proper manner for the pulses needed by the inverter. A specific block must be added also after the fuzzy controller in order to realize its triggering 0 - 1 (fig. 10).



Figures 8: Acquisition block for the current NFC training.



Figures 9: A local image of the current training data.



Figures 10: The current NFCs with its elements.

A comparison between the initial commutations of the current controller and those after a selection procedures of samples (division by 5) shows that this kind of data preparing could totally change the commutation regime of the inverter:

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1 0

1

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1

- 1
- $\begin{array}{ccc} 0 & 0 \\ 1 & 0 \end{array}$

0

A test with the tuned speed NFC inserted in a system having the current NFCc was made and the results are encouraging - fig. 11. More, the "coexistence" of both NFCs (speed and 3 x current) seems not having some bad effects on the input-output variable evolution for the speed controller - see fig. 12a (only the speed controller is a NF type) and b (both speed and current controllers are NF type).





CONCLUSIONS

The author was interested in obtaining a robust vector control for asynchronous motors by means of neurofuzzy controllers both for the speed and the current loops. The interesting aspects of the research (and the challenge too) concern the passing from a simple controller (with a few or even a single tuning parameter) to a much more complex controller, the neuro-fuzzy units having, practically, an infinite tuning parameters. Although are available methods and programs able to deliver neuro-fuzzy controller based on training input output data, the designer must pay a special attention to some important aspects: the most relevant operating conditions / regimes for the training data acquisition, the pre-processing of these data (by selection, filtering), the training parameters (epochs number, fuzzy sets as number and type etc and, finally, a post-tuning of the neuro-fuzzy controller. A double-input-single output neuro-fuzzy controller is able to bring better results for the system, in term of a solid robustness for different operating conditions. The design of the current neurofuzzy controller is much more complex because of the request to having the output in commutation for driving the power inverter. It is important to mention that the synthesis of a neuro-fuzzy controller operating in commutation mode is possible but requires additional blocks and must be made with lot of care. The tuning of the N-F controllers consists, in fact, in the choice of the fuzzy sets number, their distribution, the operator type and the selected defuzzification method. Some tests with several values for the epochs number proved a minor or no visible influence on the results in term of the training method error. Their number, however, could influence directly the surface control surface and, by that, some accuracy details of the system behavior. The influence of the AND/OR operators was not detectable in the shape of the surface control. The most important difference in the results validity comes from the IN-OUT training data that have a major influence on the distribution of the fuzzy sets; very seldom they have an uniform distribution. Also, different motor parameter sets generate N-F controller having very distinctive characteristics.

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Figures 12: The In - Out evolution (local) for the DISO optimized speed NFC in conjunction with current NFC.

SMALL SPEED ASYMPTOTIC STABILITY STUDY OF AN INDUCTION MOTOR SENSORLESS SPEED CONTROL SYSTEM WITH EXTENDED GOPINATH OBSERVER

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KEYWORDS

Extended Gopinath observer; induction motor, vector control system, direct rotor flux orientation method, asymptotic stability, sensorless.

ABSTRACT

In this paper presents synthesis extended Gopinath observer (EGO) and analyzes the asymptotic stability of a vector control system for a squirrel-cage induction motor that contains in its loop an EGO. The studied control system is based on the direct rotor flux orientation method (DFCO) and the stability study is based upon the linearization theorem around the equilibrium points of the control system, emphasizing the estimated variation domain of the rotor resistance for which the control system remains asymptotically stable when the prescribed speed of the control system is close to zero. The stability study is made in continual case. The mathematical model of the vector regulating system is made using a value $d\lambda_e - q\lambda_e$ linked to stator current.

INTRODUCTION

This paper presents a new flux and rotor speed observer called an Extended Gopinath observer (EGO). The design of the EGO observer is done based on an adaptive mechanism using the notion of Popov hyperstability (Popov 1973).

Thus, this type of observer is included in the estimation methods based on an adaptation mechanism, along with the Extended Luenberger Observer (ELO) proposed by Kubota (Kubota et al. 1990) and the Model Adaptive System (MRAS) observer proposed by Schauder (Schauder 1992).

In the second part of the paper a study is made about the asymptotic stability of the whole speed control system which contains in his loop an EGO estimator.

THE GOPINATH EXTENDED OBSERVER

The EGO observer in composed of Gopinath rotor flux observer and adaptation mechanism used for the rotor speed estimation.

The equations that define the rotor flux Gopinath observer are (Pana 2001):

$$\begin{cases} \frac{d}{dt}\hat{i}_{s} = a_{11}^{*}\cdot\underline{i}_{s} + a_{12}^{*}\cdot\underline{\psi}_{r} + b_{11}^{*}\cdot\underline{u}_{s} \\ \frac{d}{dt}\underline{\psi}_{r} = a_{21}^{*}\cdot\underline{i}_{s} + a_{22}^{*}\cdot\underline{\psi}_{r} + \underline{g}\cdot\left[\frac{d}{dt}\underline{i}_{s} - \frac{d}{dt}\hat{i}_{s}\right] \end{cases}$$
(1)

where:

$$\begin{split} a_{11}^{*} &= -\left(\frac{1}{T_{s}^{*} \cdot \sigma^{*}} + \frac{1 - \sigma^{*}}{T_{r}^{*} \cdot \sigma^{*}}\right); a_{12}^{*} = a_{13}^{*} - j \cdot a_{14}^{*} \cdot z_{p} \cdot \hat{\omega}_{r}; \\ a_{13}^{*} &= \frac{L_{m}^{*}}{L_{s}^{*} \cdot L_{r}^{*} \cdot T_{r}^{*} \cdot \sigma^{*}}; a_{14}^{*} = \frac{L_{m}^{*}}{L_{s}^{*} \cdot L_{r}^{*} \cdot \sigma^{*}}; a_{21}^{*} = a_{31}^{*}; a_{31}^{*} = \frac{L_{m}^{*}}{T_{r}^{*}} \\ a_{22}^{*} &= a_{33}^{*} + j \cdot z_{p} \cdot \hat{\omega}_{r}; a_{33}^{*} = -\frac{1}{T_{r}^{*}}; b_{11}^{*} = \frac{1}{L_{s}^{*} \cdot \sigma^{*}}; T_{s}^{*} = \frac{L_{s}^{*}}{R_{s}^{*}}; \\ T_{r}^{*} &= \frac{L_{r}^{*}}{R_{r}^{*}}; \ \sigma^{*} = 1 - \frac{\left(L_{m}^{*}\right)^{2}}{L_{s}^{*} \cdot L_{r}^{*}}. \end{split}$$

In the above relations (1) marked with "*" the identified electrical sizes of the induction engine.

The block diagram of the EGO is presented in figure 1



Figure 1: The Principle Schematic of the EGO Estimator

The essential element that determines the flux observer's stability, and also his lack of sensibility to the engine's parameters variation, is a g gate, which is a complex number of the form: $g = g_a + j \cdot g_b$.

In order to design this type of estimator we need to position the estimator's poles in the left Nyquist plane so that the estimator's stability is asured. The expressions g_a and g_b after the pole positioning are (Pana 2001):

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$$\begin{cases} g_a = \frac{1}{a_{14}^*} \cdot \left[\frac{\widehat{\omega}_r \cdot z_p \cdot \beta - \alpha \cdot a_{33}^*}{\left(\widehat{\omega}_r \cdot z_p \right)^2 + \left(a_{33}^* \right)^2} - 1 \right] \\ g_b = \frac{\widehat{\omega}_r \cdot z_p \cdot \alpha + a_{33}^* \cdot \beta}{\left(\widehat{\omega}_r \cdot z_p \right)^2 + \left(a_{33}^* \right)^2} \cdot \frac{1}{a_{14}^*} \end{cases}$$
(2)

The optimum position of the poles, the α and β values respectively, are obtained by the minimization of the induction motor's rotor resistance variation over the stability of the flux observer. We get the following (Pana 2001):

$$\beta = 0; \alpha = k \cdot \sqrt{\left(\widehat{\omega}_r \cdot z_p\right)^2 + \left(a_{33}^*\right)^2}; k > 0$$
(3)

In these conditions the Gopinath rotor flux observer is completely determined.

Next, in order to determine the adaptation mechanism used to estimate the rotor speed, we will consider as a reference model the "stator curents - rotor fluxes" model of the induction engine and as an ajustable model, the model of the Gopinath rotor flux observer. The equations mentioned above written under the input-state-output canonic form are:

Reference model:

$$\begin{cases} \frac{d}{dt}x = A \cdot x + B \cdot u \\ y = C \cdot \frac{d}{dt}x \end{cases}$$
(4)

• Ajustable model:

$$\begin{cases} \frac{d}{dt}\hat{x} = \tilde{A}\cdot\hat{x} + A_{1}\cdot x + B\cdot u + \tilde{G}\cdot(y-\hat{y}) \\ \hat{y} = C\cdot\frac{d}{dt}\hat{x} \end{cases}$$
(5)

where:

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}; \widetilde{A} = \begin{bmatrix} 0 & a_{12}^* \\ 0 & a_{22}^* \end{bmatrix}; A_1 = \begin{bmatrix} a_{11}^* & 0 \\ a_{21}^* & 0 \end{bmatrix}; \widetilde{G} = \begin{bmatrix} 0 \\ \underline{g} \end{bmatrix}$$
$$x = \begin{bmatrix} \underline{i}_s \\ \underline{\psi}_r \end{bmatrix}; \widehat{x} = \begin{bmatrix} \hat{i}_s \\ \underline{\hat{\psi}}_r \end{bmatrix}; u = \underline{u}_s; B = \begin{bmatrix} b_{11} \\ 0 \end{bmatrix}; C = \begin{bmatrix} 1 & 0 \end{bmatrix}.$$

In the above relations we marked with "~" the Gopinath estimator's matrices which are dependent upon the rotor speed, which in turn needs to be estimated based on the adaptation mechanism.

Next, in order to determine the expression that defines the adaptation mechanism we will asume that the identified electric sizes are identical with the real electric sizes of the induction engine.

In other words: $a_{ij} = a_{ij}^*$; i, j = 1, 2 and $b_{11} = b_{11}^*$

In order to build the adaptive mechanism, for start we will calculate the estimation error given by the difference:

$$e_{\chi} = x - \hat{x} \tag{6}$$

Derivation the relation (6) in relation with time and by using the relations (4) and (5) the relation (6) becomes:

$$\frac{d}{dt}e_{\mathbf{X}} = (A - A_{\mathbf{I}}) \cdot \mathbf{x} - \widetilde{A} \cdot \hat{\mathbf{x}} - \widetilde{G} \cdot C \cdot \frac{d}{dt}e_{\mathbf{X}}$$
(7)

If the determinant, $\det(I_2 + \widetilde{G} \cdot C) \neq 0$, then it exists a unique inverse matrix $M = (I_2 + \widetilde{G} \cdot C)^{-1}$ so that the expression (7) can be written like this:

$$\frac{d}{dt}e_{\chi} = M \cdot (A - A_{1}) \cdot e_{\chi} + M \cdot (A - A_{1} - \widetilde{A}) \cdot \hat{x}$$
(8)

Equation (8) describes a linear system defined by the term $M \cdot (A - A_1) \cdot e_x$ in inverse connection with a non linear system defined by the term $\Phi(e_y)$ which receives at input the error $e_y = C \cdot e_x$ between the models and has at the output the term:

$$\rho = -M \cdot \left(A - A_{\rm l} - \tilde{A} \right) \cdot \hat{x} \tag{9}$$

The block diagram of the system that describes the dynamic evolution of the error between the state of the reference model and the state of the adjustable model is presented in figure 2:



Figure 2: The block diagram of the system that describes the dynamic evolution of the error between the state of teh reference model and the state of the adjustable model

As one may notice, this problem is frequently treated in the literature of the non-linear systems, being exactly the configuration of the Lure problem, and of one of the problems treated by Popov.

Considering, according to the Popov terminology, the non-linear block described by $\Phi(e_y)$ the integral inputoutput index associated to it is:

$$\eta(t_0, t_1) = \operatorname{Re}\left[\int_0^{t_1} e_y^T(t) \cdot \rho(t) dt\right]$$
(10)

In order for block to be hyper-stable a necessary condition is:

$$\eta(0,t_1) = \operatorname{Re}\left[\int_0^{t_1} e_y^T(t) \cdot \rho(t) dt\right] \ge -\gamma^2(0) \quad (11)$$

for any input-output combination and where $\gamma(0)$ is a positive constant.

In the above relation we marked with e_y^T the following expression

$$\boldsymbol{e}_{\boldsymbol{y}}^{T} = \begin{bmatrix} \bar{\boldsymbol{e}}_{\boldsymbol{y}} & \boldsymbol{0} \end{bmatrix}$$
(12)

Obtained in order to keep the compatibility between the input and output dimensions, and $\overline{e_y}$ represents the conjugate of the complex variable e_y .

Under these circumstances, using the relation (9) the expression (11) becomes:

$$\eta(0,t_1) = -\operatorname{Re}\left[\int_0^{t_1} e_{y}^{T}(t) \cdot M \cdot \left(A - A_1 - \widetilde{A}\right) \cdot \widehat{x} dt\right] \ge -\gamma^2(0) \quad (13)$$

Next we assume that the error $M \cdot (A - A_1 - \widetilde{A})$ is determined only by the rotor speed of the induction machine. In this case we may write:

$$M \cdot \left(A - A_{\rm I} - \widetilde{A}\right) = \left(\omega_r - \widehat{\omega}_r\right) \cdot A_{er} \tag{14}$$

where: $A_{er} = \begin{bmatrix} 0 & -j \cdot a_{14} \cdot z_p \\ 0 & j \cdot z_p \cdot (1 + a_{14} \cdot \underline{g}) \end{bmatrix}$.

For any positive derivable f function we can demonstrate the following inequality:

$$K_1 \cdot \int_0^{t_1} \left(\frac{df}{dt} \cdot f\right) dt \ge -\frac{K_1}{2} \cdot f^2\left(0\right) \qquad (15)$$

On the other hand, using the relation (14), the expression (13) becomes:

$$\eta(0,t_1) = -\operatorname{Re}\left\{\int_0^{t_1} \left[e_y^T(t) \cdot A_{er} \cdot \hat{x} \cdot \left(\omega_r - \hat{\omega}_r\right) \right] dt \right\} \ge -\gamma^2(0) \quad (16)$$

By combining the relations (15) and (16) we can write the following relations:

$$\begin{cases} f = \omega_r - \hat{\omega}_r \\ -\operatorname{Re}\left(e_y^T \cdot A_{er} \cdot \hat{x}\right) = K_1 \cdot \frac{df}{dt} \end{cases}$$
(17)

Because K_1 is a constant and then, in case of a slower ω_r parameter variation related to the adaptive law, we can write:

$$\widehat{\omega}_r = k_i \cdot \int \operatorname{Re}\left(e_v^T \cdot A_{er} \cdot \hat{x}\right) dt \tag{18}$$

After replacing the variables that define the above expression (18) and taking into account the arbitrary nature of the K_i positive constant we obtain:

$$\widehat{\omega}_r = k_i \cdot \int \left(e_{yd} \cdot \widehat{\psi}_{qr} - e_{yq} \cdot \widehat{\psi}_{dr} \right) dt \qquad (19)$$

where $e_{yd} = i_{ds} - \hat{i}_{ds}$ and $e_{yq} = i_{qs} - \hat{i}_{qs}$.

Sometimes, insted of the adaptation law (19) we can use the following form:

$$\hat{\omega}_{r} = K_{R} \left(e_{yd} \cdot \hat{\psi}_{qr} - e_{yq} \cdot \hat{\psi}_{dr} \right) + k_{i} \cdot \int \left(e_{yd} \cdot \hat{\psi}_{qr} - e_{yq} \cdot \hat{\psi}_{dr} \right) dt$$
(20)

From the above relation we ca observe that a new proportional component apears from the desire to have 2 coefficients that can control the speed estimation dynamics. This fact isn't always necessary because we can obtain very good results by using only expression (19).

Thus expression (20) represents the general formula of the adaptation mechanism where K_R represents the proportionality constant and $K_i = K_R/T_R$; where T_R represents the integration time of the proportional-integral regulator that defines the adaptation mechanism.

THE MATHEMATICAL DESCRIPTION OF THE VECTOR CONTROL SYSTEM

The block diagram of the control system of the mechanical angular speed ω_r of the induction engine with a discrete orientation after the rotor flux (DFOC) is presented in figure 3.



Figure 3: The block diagram of the DFCO vectorial control system which contains an EGO loop.

In figure 3 we marked with B2 the control block of the speed control system with direct orientation after the rotor flux (DFCO) and with B1 the extended Gopinath estimator block (EGO).

In order to mathematically describe the DFOC control system the following hypotheses have been considered:

- The static frequency converter (CSF) is assumed to contain a tension inverter.
- The static frequency converter is considered ideal so that the vector of the command measures is considered to be the entry vector of the induction motor.
- The dynamic measure transducers are considered ideal.
- The mathematical model of the vector control system will be written in an $d\lambda_e q\lambda_e$ axis reference bounded to the stator current.

Some of the equations that define the vector control system are given by the elements which compose the field orientation block and consist of:

• Stator tensions decoupling block (C₁U_s):

$$\begin{cases} u_{aba}^{*} = \frac{1}{b_{11}^{*}} \cdot \left[b_{11}^{*} \cdot v_{aba}^{*} - a_{13}^{*} \cdot |\psi_{r}| - a_{31}^{*} \cdot \frac{i_{gab}^{2}}{|\psi_{r}|} - z_{p} \cdot \hat{\omega}_{b} \cdot i_{gab} \right] \\ u_{gab}^{*} = \frac{1}{b_{11}^{*}} \cdot \left[b_{11}^{*} \cdot v_{gab}^{*} + a_{14}^{*} \cdot z_{p} \cdot \hat{\omega}_{b} \cdot |\psi_{r}| + a_{31}^{*} \cdot \frac{i_{dab}^{*} \cdot i_{gab}}{|\psi_{r}|} + z_{p} \cdot \hat{\omega}_{b} \cdot i_{dab} \right] \end{cases}$$
(21)

• PI flux regulator (PI_ ψ) defined by the K_{ψ} proportionality constant and the T_{ψ} integration time:

$$\begin{cases} \frac{dx_6}{dt} = \psi_r^* - |\psi_r| \\ i_{ds\lambda_r}^* = \frac{K_{\psi}}{T_{\psi}} \cdot x_6 + K_{\psi} \cdot (\psi_r^* - |\psi_r|) \end{cases}$$
(22)

couple PI regulator (PI_M_e) defined by the K_M proportionality constant and the T_M integration time:

$$\begin{cases} \frac{dx_{\gamma}}{dt} = M_e^* - M_e \\ i_{qs\lambda_r}^* = \frac{K_M}{T_M} \cdot x_{\gamma} + K_M \cdot \left(M_e^* - M_e\right) \end{cases}$$
(23)

mechanical angular speed PI regulator (PI_W) defined by the K_ω proportionality constant and the T_α integration time:

$$\begin{cases} \frac{dx_8}{dt} = \omega_r^* - \hat{\omega}_r \\ M_e^* = \frac{K_{\omega}}{T_{\omega}} \cdot x_8 + K_{\omega} \cdot \left(\omega_r^* - \hat{\omega}_r\right) \end{cases}$$
(24)

current PI regulator (PI_I) defined by the K_i proportionality constant and the T_i integration time:

$$\begin{cases} \frac{dx_{9}}{dt} = i_{ds\lambda_{r}}^{*} - i_{ds\lambda_{r}} \\ v_{ds\lambda_{r}}^{*} = \frac{K_{i}}{T_{i}} \cdot x_{9} + K_{i} \cdot \left(i_{ds\lambda_{r}}^{*} - i_{ds\lambda_{r}}\right) \end{cases}$$

$$\begin{cases} \frac{dx_{10}}{dt} = i_{qs\lambda_{r}}^{*} - i_{qs\lambda_{r}} \\ v_{qs\lambda_{r}}^{*} = \frac{K_{i}}{T_{i}} \cdot x_{10} + K_{i} \cdot \left(i_{qs\lambda_{r}}^{*} - i_{qs\lambda_{r}}\right) \end{cases}$$

$$(25)$$

• Flux analyzer (AF):

$$\begin{cases} |\psi_r| = \sqrt{\widehat{\psi}_{dr}^2 + \widehat{\psi}_{qr}^2} \\ \sin \lambda_r = \frac{\widehat{\psi}_{qr}}{|\psi_r|}; \cos \lambda_r = \frac{\widehat{\psi}_{dr}}{|\psi_r|} \end{cases}$$
(27)

• The calculate of the couple block (C₁M_e):

$$M_e = K_a \cdot \left| \psi_r \right| \cdot i_{qs\lambda_r} \tag{28}$$

The other equations that define the mathematic model of the speed's vector control system are:

• The equations that define the stator currents – rotor fluxes mathematical model of the induction engine; 4 equations defined based on the first relation in the canonic system (4) to which we can add the induction machine's motion equation defined by the following expression:

$$\frac{d}{dt}\omega_r = K_{m_1} \cdot \left[\psi_{dr} \cdot i_{qs} - \psi_{qr} \cdot i_{ds}\right] - K_{m_2} \cdot \omega_r - K_{m_3} \cdot M_r \quad (29)$$

where: $K_{m_1} = \frac{3}{2} \cdot \frac{z_p}{J} \cdot \frac{L_m}{L_r}$; $K_{m_2} = \frac{F}{J}$; $K_{m_3} = \frac{1}{J}$.

• The equations that define the extended Gopinath observer defined by the 4 relations that can be written based on system (1) with the equation that defines the speed adaptation mechanism (20). Expression (20) can also be written like below:

$$\begin{cases} \frac{d}{dt} x_{15} = (\dot{i}_{ds} - \hat{i}_{ds}) \cdot \hat{\psi}_{qr} - (\dot{i}_{qs} - \hat{i}_{qs}) \cdot \hat{\psi}_{dr} \\ \hat{\omega}_{r} = \frac{K_{R}}{T_{R}} \cdot x_{15} + K_{R} \cdot \left[(\dot{i}_{ds} - \hat{i}_{ds}) \cdot \hat{\psi}_{qr} - (\dot{i}_{qs} - \hat{i}_{qs}) \cdot \hat{\psi}_{dr} \right] \end{cases}$$
(30)

All these expressions form a 15 differential equations system with 15 unknown values. In order to offer a

coherent presentation of this differential equations system, we have used the following notations:

• The state vector of the control system will be

$$x = \left[x_i\right]_{i=\overline{1,15}} \tag{31}$$

where: $x_1 = i_{ds\lambda_e}$; $x_2 = i_{qs\lambda_e}$; $x_3 = \psi_{dr\lambda_e}$; $x_4 = \psi_{qr\lambda_e}$; $x_5 = \omega_r$; $x_{11} = \hat{i}_{ds\lambda_e}$; $x_{12} = \hat{i}_{qs\lambda_e}$; $x_{13} = \hat{\psi}_{dr\lambda_e}$; $x_{14} = \hat{\psi}_{qr\lambda_e}$. • The input vector of the of the control system will be

$$u = \begin{bmatrix} u_1 & u_2 & u_3 \end{bmatrix}^T \tag{32}$$

where: $u_1 = \psi_r^*$; $u_2 = \omega_r^*$; $u_3 = M_r$.

Under these circumstances the 15 differential equations system that define the mathematical model of the vector regulating system can be written as follows

$$\frac{d}{dt}x = f(x,u) \tag{33}$$

where: $f(x,u) = [f_i(x,u)]_{i=\overline{1,15}}$ and the $f_i = f_i(x,u)$ functions are:

$$f_1(x,u) = a_{11} \cdot x_1 + \omega_e \cdot x_2 + a_{13} \cdot x_3 + a_{14} \cdot z_p \cdot x_5 \cdot x_4 + b_{11} \cdot u_a$$
(34)

$$f_2(x,u) = -\omega_e \cdot x_1 + a_{11} \cdot x_2 - a_{14} \cdot z_p \cdot x_5 \cdot x_3 + a_{13} \cdot x_4 + b_{11} \cdot u_b$$
(35)

$$f_3(x,u) = a_{31} \cdot x_1 + a_{33} \cdot x_3 + (\omega_e - z_p \cdot x_5) \cdot x_4$$
(36)

$$f_4(x,u) = a_{31} \cdot x_2 - (\omega_e - z_p \cdot x_5) \cdot x_3 + a_{33} \cdot x_4$$
(37)

$$f_5(x,u) = K_{m_1} \cdot [x_3 \cdot x_2 - x_4 \cdot x_1] - K_{m_2} \cdot x_5 - K_{m_3} \cdot u_3 \quad (38)$$

$$f_6(x,u) = u_1 - g_1 \tag{39}$$

$$f_7(x,u) = \frac{K_{\omega}}{T_{\omega}} \cdot x_8 + K_{\omega} \cdot (u_2 - g_2) - K_a \cdot g_3$$
(40)

$$f_8(x,u) = u_2 - g_2 \tag{41}$$

$$f_{9}(x,u) = \frac{K_{\psi}}{T_{\psi}} \cdot x_{6} + K_{\psi} \cdot (u_{1} - g_{1}) - \frac{g_{4}}{g_{1}}$$
(42)

$$f_{10}(x,u) = \frac{K_M}{T_M} \cdot x_7 + K_M \cdot f_7(x,u) - \frac{g_3}{g_1}$$
(43)

 $f_{11}(x,u) = a_{11}^* \cdot x_1 + \omega_e \cdot x_2 + a_{13}^* \cdot x_{13} + a_{14}^* \cdot z_p \cdot g_2 \cdot x_{14} + b_{11}^* \cdot u_a$ (44) $f_{12}(x,u) = -\omega_e \cdot x_1 + a_{11}^* \cdot x_2 - a_{14}^* \cdot z_n \cdot g_2 \cdot x_{13} + a_{13}^* \cdot x_{14} + b_{11}^* \cdot u_h$ (45)

$$f_{13}(x,u) = b_1 \cdot x_{13} + b_2 \cdot x_{14} - g_a \cdot b_{11}^* \cdot u_a + g_b \cdot b_{11}^* \cdot u_b + + b_3 \cdot x_1 + b_4 \cdot x_2 + g_a \cdot f_1(x,u) - g_b \cdot f_2(x,u)$$
(46)

$$f_{14}(x,u) = -b_2 \cdot x_{13} + b_1 \cdot x_{14} - g_b \cdot b_{11}^* \cdot u_a - g_a \cdot b_{11}^* \cdot u_b - -b_4 \cdot x_1 + b_3 \cdot x_2 + g_b \cdot f_1(x,u) + g_a \cdot f_2(x,u)$$
(47)

$$f_{15}(x,u) = (x_1 - x_{11}) \cdot x_{14} - (x_2 - x_{12}) \cdot x_{13}$$
(48)

where:

$$\begin{split} g_{1} &= \sqrt{x_{13}^{2} + x_{14}^{2}}; \\ g_{2} &= \frac{K_{R}}{T_{R}} \cdot x_{15} + K_{R} \cdot \left[(x_{1} - x_{11}) \cdot x_{14} - (x_{2} - x_{12}) \cdot x_{13} \right]; \\ g_{3} &= x_{2} \cdot x_{13} - x_{1} \cdot x_{14}; g_{4} &= x_{1} \cdot x_{13} + x_{2} \cdot x_{14}; \\ b_{1} &= a_{33}^{*} - g_{a} \cdot a_{13}^{*} - g_{b} \cdot a_{14}^{*} \cdot z_{p} \cdot g_{2}; \\ b_{2} &= g_{b} \cdot a_{13}^{*} - \left(1 + g_{a} \cdot a_{14}^{*} \right) \cdot z_{p} \cdot g_{2} + \omega_{e}; \\ b_{3} &= a_{31}^{*} - g_{a} \cdot a_{11}^{*} - g_{b} \cdot \omega_{e}; b_{4} &= g_{b} \cdot a_{11}^{*} - g_{a} \cdot \omega_{e}; \\ \phi_{e} &= z_{p} \cdot g_{2} + a_{31}^{*} \cdot \frac{x_{2}}{x_{13}}; \\ \alpha &= k \cdot \sqrt{\left(g_{2} \cdot z_{p}\right)^{2} + \left(a_{33}^{*}\right)^{2}}; \\ g_{a} &= \frac{-1}{a_{14}^{*}} \cdot \left[1 + \frac{\alpha \cdot a_{33}^{*}}{\left(g_{2} \cdot z_{p}\right)^{2} + \left(a_{33}^{*}\right)^{2}} \right]; \\ g_{b} &= \frac{g_{2} \cdot z_{p} \cdot \alpha}{\left(g_{2} \cdot z_{p}\right)^{2} + \left(a_{33}^{*}\right)^{2}} \cdot \frac{1}{a_{14}^{*}}; \\ v_{a} &= \frac{K_{i}}{T_{i}} \cdot x_{9} + K_{i} \cdot f_{9}(x, u); v_{b} &= \frac{K_{i}}{T_{i}} \cdot x_{10} + K_{i} \cdot f_{10}(x, u); \\ h_{1} &= a_{13}^{*} \cdot g_{1} - a_{31}^{*} \cdot \frac{g_{3}^{2}}{g_{1}^{3}} - z_{p} \cdot g_{2} \cdot \frac{g_{3}}{g_{1}}; \\ h_{2} &= a_{14}^{*} \cdot z_{p} \cdot g_{2} \cdot g_{1} + a_{31}^{*} \cdot \frac{g_{3} \cdot g_{4}}{g_{1}^{3}} + z_{p} \cdot g_{2} \cdot \frac{g_{4}}{g_{1}}; \\ u_{a} &= \frac{1}{b_{11}^{*} \cdot g_{1}} \cdot \left[x_{14} \cdot \left(b_{11}^{*} \cdot v_{a} - h_{1}\right) - x_{14} \cdot \left(b_{11}^{*} \cdot v_{b} + h_{2}\right) \right]; \\ u_{b} &= \frac{1}{b_{11}^{*} \cdot g_{1}} \cdot \left[x_{14} \cdot \left(b_{11}^{*} \cdot v_{a} - h_{1}\right) + x_{13} \cdot \left(b_{11}^{*} \cdot v_{b} + h_{2}\right) \right]. \\ a_{11} &= -\left(\frac{1}{T_{s} \cdot \sigma} + \frac{1 - \sigma}{T_{r} \cdot \sigma} \right); a_{13} = \frac{L_{m}}{L_{s} \cdot L_{r} \cdot T_{r} \cdot \sigma}; \\ a_{14} &= \frac{L_{m}}{L_{s} \cdot L_{r} \cdot \sigma}; a_{31} = \frac{L_{m}}{T_{r}}; a_{33} = -\frac{1}{T_{r}}; b_{11} = \frac{1}{L_{s} \cdot c_{r}}; \frac{L_{m}^{*}}{T_{r}}; \\ x_{s} &= \frac{1}{R_{s}}; T_{r} = \frac{L_{r}}{R_{s}}; T_{r} = \frac{L_{r}}{R_{r}}; \sigma = 1 - \frac{L_{m}^{2}}{L_{s} \cdot L_{r}}; K_{a} = \frac{3}{2} \cdot z_{p} \cdot \frac{L_{m}^{*}}{T_{r}}. \end{cases}$$

Under these circumstances the mathematical model of the speed vector control system is fully determined as being defined by the non-linear differential equations system given by (33) whose initial condition is x(0) = 0.

THE ASYMPTOTIC STABILITY STUDY OF THE CONTROL SYSTEM

In order to realize the analysis of the asymptotic stability an induction with the following parameters has been considered:

• Electrical parameters

$$\begin{split} R_s &= 0.371 \left[\Omega \right]; \ R_r = 0.415 \left[\Omega \right]; \ L_s = 0.08694 \left[\mathrm{H} \right]; \\ L_r &= 0.08762 \left[\mathrm{H} \right]; \ L_m = 0.08422 \left[\mathrm{H} \right]. \end{split}$$

Mechanical parameters

$$z_p = 2$$
; $J = 0.15 \left[\text{kg} \cdot \text{m}^2 \right]$; $F = 0.005 \left[\frac{\text{N} \cdot \text{m} \cdot \text{s}}{\text{rad}} \right]$

On the other hand, following the automated regulators' tuning within the speed control system the following constants have been obtained:

$$\begin{split} K_{\psi} &= 501.3834 \ ; T_{\psi} = \frac{K_{\psi}}{2374.7} \ ; K_i = 5.9881 \ ; T_i = \frac{K_i}{754.4176} \ ; \\ K_M &= 10.1988 \ ; \ T_M = \frac{K_M}{1020} \ ; K_{\omega} = 10 \ ; \ T_{\omega} = \frac{K_{\omega}}{350} \ ; \\ K_R &= 6 \ ; \ T_R = \frac{K_R}{4000} \ . \end{split}$$

In the relations above, K_R represents the proportionality constant and T_R represents the integration time of the PI regulator from the speed estimator designed based on the Popov hyperstability.

Under these circumstances by imposing the entry vector of the control system to be of the following type

$$u_{1} = \psi_{r}^{*} = 0.69 \, [\text{Wb}]; u_{2m} = \omega_{rm}^{*} = n_{m} \cdot \frac{\pi}{30} \left[\frac{\text{rad}}{\text{s}} \right];$$
$$u_{3} = M_{r} = M_{N} = 93.269 \, [\text{N} \cdot \text{m}]$$
(49)

where $n_m = 100 \cdot m$ [rpm] with $m = \overline{0, 15}$ and the proportionality coefficient k = 1.3 by solving the non-linear system

$$f(x,u) = 0 \tag{50}$$

Using the Newton method having as the start point the vector

$$x^* = \begin{bmatrix} 0 & 0 & u_1 & 0 & u_{2m} & 0 & 0 & 0 & 0 & 0 & 0 & u_1 & 0 & 0 \end{bmatrix}^T (51)$$

The equilibrium point $x_m = b_m$ results, where $b_m = [b_{mi}]_{i=\overline{1,15}}$.

From those stated above by the linearization of the system (33) around the equilibrium point $x_m = b_m$

obtained for an $u^* = \begin{bmatrix} u_1 & u_{2m} & u_3 \end{bmatrix}^T$ entry vector defined by (49) we get:

$$\Delta \dot{x}(t) = A_L \cdot \Delta x(t) + B_L \cdot \Delta u(t)$$
(52)

where A_L, B_L matrixes are

$$A_{L} = \left[\frac{\partial f_{i}}{\partial x_{j}}(b_{m}, u^{*})\right]_{i=\overline{1,15}; j=\overline{1,15}}; B_{L} = \left[\frac{\partial f_{i}}{\partial u_{k}}(b_{m}, u^{*})\right]_{i=\overline{1,15}; k=\overline{1,3}}.$$

Next, in order to study the asymptotic stability of the equilibrium points $x_m = b_m$, the eigenvalues of the A_L matrix will be analyzed, so that if they have a strictly negative real part the $x_m = b_m$ equilibrium point is asymptotically stable for the linerized system (52). Under these circumstances according to the linearization theorem (Voicu 1986) in a vicinity of the equilibrium point $x_m = b_m$ the non-linear system (33) is asymptotically stable. As the eigenvalues of the A_L matrix are presented within Figure 4, it results that the equilibrium points $x_m = b_m$ of the linerized system (52) are asymptotically stable and according to the linearization theorem the equilibrium points $x_m = b_m$ are asymptotically stable in certain vicinity for the non-linear system (33).



Figure 4. The eigenvalues of the matrix A_L ; $M_r = M_N$

For a more detailed study of the asymptotic stability, next we will present the A_L matrix eigenvalues under identical testing conditions with those above with the difference that $u_3 = M_r = M_N = 0 [N \cdot m]$. As with the previous case from Figure 5 one may notice that the $x_m = b_m$ equilibrium points of the linerized system are asymptotically stable resulting that in certain

vicinity these points are asymptotically stable for the non-

linear system defined by (33).



Figure 5. The eigenvalues of the matrix A_L ; $M_r = 0$

Next, the influence of the estimated rotor resistance will be emphasized, when studying asymptotic stability of the equilibrium point $x_0 = b_0$ of the non-linear system (33) in a certain vicinity of this point.

The equilibrium point is obtained for an entry vector like $u = \begin{bmatrix} u_1 & u_{20} & u_3 \end{bmatrix}^T$ defined by (49); namely for a speed of $n_0 = 0$ [rpm].

Based on this study we can obtain information related to the range of variation of the estimated rotor resistance for which the non-linear system (33) remains asymptotically stable around the $x_0 = b_0$ equilibrium point.

As the eigenvalues of the A_L matrix are presented in figure 6, it results that the non-linear system (33) around the equilibrium point $x_0 = b_0$ is asymptotically stable for an estimated rotor resistance in range of $D_1 = \{R_r^*; 0.6 \cdot R_r \le R_r^* \le 2.28 \cdot R_r\}$, becoming asymptotically unstable for an estimated rotor resistance in range of $D_2 = \{R_r^*; 2.28 \cdot R_r < R_r^* < 0.6 \cdot R_r\}$.



Figure 6. A_L Eigenvalues by rotor resistance for $n_0 = 0[rpm]; M_r = M_N$

Next the influence of the estimated rotor resistance to the asymptotic stability of the non-linear system (33) will be presented, when the entry vector is $u = \begin{bmatrix} u_1 & u_{20} & u_3 \end{bmatrix}^T$ defined by (49) with the difference that $u_3 = M_r = M_N = 0 [N \cdot m]$. The eigenvalues of the A_L matrix are presented in Figure 7.



Figure 7. A_L eigenvalues by rotor resistance for $n_0 = 0[rpm]; M_r = 0$

As the eigenvalues of the A_L matrix are presented in figure 7, it results that the non-linear system (33) around the equilibrium point $x_0 = b_0$ is asymptotically stable for an estimated rotor resistance in range of $D_1 = \{R_r^*; 0.1 \cdot R_r \le R_r^* \le 2.289 \cdot R_r\}$, becoming asymptotically unstable for an estimated rotor resistance in range of $D_2 = \{R_r^*; 2.289 \cdot R_r < R_r^* < 0.1 \cdot R_r\}$.

On the other hand in case we perform the digitization of the linear system (22) we get:

$$x(k+1) = F_L \cdot x(k) + H_L \cdot u(k)$$
(53)

where: the F_L , H_L matrixes are obtained from the A_L , B_L matrixes using one of the two digitization types:

Simplified digitization:

$$F_L = I_{15} + A_L \cdot T ; \quad H_L = B_L \cdot T \tag{54}$$

• Complete digitization:

$$F_{L} = I_{15} + A_{L} \cdot T + A_{L}^{2} \cdot \frac{T^{2}}{2}; \quad H_{L} = B_{L} \cdot T + A_{L} \cdot B_{L} \cdot \frac{T^{2}}{2} \quad (55)$$

with the sampling time T.

Proceeding in a similar manner the eigenvalues of the F_L matrix in case the entry vector is defined by (49) and the F_L matrix is obtained by using simplified digitization using a $T = 53.3 [\mu \text{ sec}]$ sampling time are graphically presented in Figure 8.


Figure 8: The eigenvalues of the F_L ; $M_r = 0$ matrix when using simplified digitization

From the figure above one may notice that the $x_m = b_m$ equilibrium points are asymptotically stable for the discrete system (53) in case the F_L matrix is obtained through using the simplified digitization method.

This conclusion also remains valid when the F_L matrix is obtained through the complete digitization method both where the resistant couple is present or absent.

Next we will present the influence of the estimated rotor resistance over the asymptotic stability of the discrete non-linear system when the entry vector is $u = \begin{bmatrix} u_1 & u_{20} & u_3 \end{bmatrix}^T$ and is defined by (49).

This study was conducted for a sampling time of $T = 53.3 [\mu \text{ sec}]$ in case of simplified digitization.

The study helped us with the information that the $x_0 = b_0$ equilibrium point remains asymptotically stable for the linear (53) system for a variation of identified rotor resistance ranging from $D_1 = \{R_r^*; 0.71 \cdot R_r \le R_r^* \le 2.272 \cdot R_r\}$.

The $x_0 = b_0$ equilibrium point becomes asymptotically unstable when the variation of the identified rotor resistance varies from $D_2 = \{R_r^*; 2.272 \cdot R_r < R_r^* < 0.71 \cdot R_r\}$



Figure 9: The eigenvalues of the F_L ; $M_r = 0$ matrix when using complete digitization

When the study of the influence of identified rotor resistance variation is done for an entry vector of the $u = \begin{bmatrix} u_1 & u_{20} & u_3 \end{bmatrix}^T$ type defined by (49) with the difference that $u_3 = M_r = M_N = 0 \begin{bmatrix} N \cdot m \end{bmatrix}$ then the stability domain for which the $x_0 = b_0$ equilibrium point is asymptotically stable is $D_1 = \{R_r^*; 0.18 \cdot R_r \le R_r^* \le 2.278 \cdot R_r\}$ and the instability domain is $D_2 = \{R_r^*; 2.278 \cdot R_r < R_r^* < 0.18 \cdot R_r\}$.

On the other hand the domains that define the upper and lower limits of variation of identified rotor resistance for which the $x_0 = b_0$ equilibrium point remains asymptotically stable for the (52) discrete linear system diminishes with the increase of the sampling time.

The results presented above have been partially proved by experiment, due to the limitations introduced by the inverter. Next, the performances of the extended Gopinath estimator are presented in a variety of functional conditions. Thus the image below will present the graphics for the real and estimated rotors fluxes and also the graphics for the imposed speed, real speed and the estimated speed for small, medium and large imposed speeds.



Figure 10: ψ_{dr} real flux compared to the $\hat{\psi}_{dr}$ estimated flux: $\omega_r^* = 5 \cdot \frac{\pi}{30} \left[\frac{\text{rad}}{\text{s}} \right]$; $M_r = 0$.



Figure 11: ω_r real speed compared to the $\hat{\omega}_r$ estimated speed and reference speed : $\omega_r^* = 5 \cdot \frac{\pi}{30} \left[\frac{\text{rad}}{\text{s}} \right]$; $M_r = 0$.



Figure 12: ψ_{dr} real flux compared to the $\hat{\psi}_{dr}$ estimated flux: $a_r^* = 1500 \cdot \frac{\pi}{30} \left[\frac{\text{rad}}{\text{s}} \right]; M_r = 0$.



Figure 13: ω_r real speed compared to the $\hat{\omega}_r$ estimated speed and reference speed: $\omega_r^* = 1500 \cdot \frac{\pi}{30} \left[\frac{\text{rad}}{\text{s}} \right]; M_r = 0$.







Figure 15: ω_r real speed compared to the $\hat{\omega}_r$ estimated speed and reference speed: $\omega_r^* = 3000 \cdot \frac{\pi}{30} \left[\frac{\text{rad}}{\text{s}} \right]; M_r = 0$.

On the other hand we will present in the following image the effect of the rotors resistance emphasizing the dynamic performances of the EGO estimator.

Thus we will present the graphic between the real and estimated rotor fluxes and also the graphic between the imposed speed, real speed and estimated speed for low, medium and high imposed speeds when the rotor resistance in at the lower limit and at the upper limit respectively, limits that separate the stability from the asymptotic instability.



Figure 16: ψ_{dr} real flux compared to the $\hat{\psi}_{dr}$ estimated flux: $\omega_r^* = 5 \cdot \frac{\pi}{2\pi} \left[\frac{\text{rad}}{2\pi} \right]$; $M_r = 0$; $R_r^* = 1.7 \cdot R_r$.

Figure 17: ω_r real speed compared to the ω_r estimated speed and reference speed: $M_r = 0$. $R_r^* = 1.7 \cdot R_r$.



Figure 18: ψ_{dr} real flux compared to the $\hat{\psi}_{dr}$ estimated flux: $\omega_r^* = 1500 \cdot \frac{\pi}{30} \left[\frac{\text{rad}}{\text{s}} \right]$; $M_r = 0 \cdot R_r^* = 1.7 \cdot R_r$.



Figure 19: ω_r real speed compared to the $\widehat{\omega}_r$ estimated speed and reference speed: $M_r = 0$; $R_r^* = 1.7 \cdot R_r$.



Figure 20: ψ_{dr} real flux compared to the $\hat{\psi}_{dr}$ estimated flux: $M_r = 0$; $R_r^* = 1.7 \cdot R_r$.



Figure 21: ω_r real speed compared to the $\hat{\omega}_r$ estimated speed and reference speed: $\omega_r^* = 3000 \cdot \frac{\pi}{30} \left[\frac{\text{rad}}{\text{s}} \right]$; $R_r^* = 1.7 \cdot R_r$.

CONCLUSIONS

This paper presents analytically in a single form the mathematical model of the speed vector-controlled system with an extended Gopinath estimator, suitable for stability analysis.

The mathematical model is written in a $d\lambda_e - q\lambda_e$ orientation value linked to the stator current vector. This mathematical model allows for both the internal asymptotic study as well as the external stability of the control system.

The study helped us to conclude that the analyzed control system is asymptotically stable for the imposed speed range (0...1500)[rpm] both, when a resistant couple is

lacking or present as $M_r = M_N$. This conclusion is valid in both the continual and discrete cases where the sampling time is $T = 53.3 [\mu \sec]$.

When the estimator from within the control system has not the same order with the motor, the estimator adds eigenvalues and affects the eigenvalues of the regulating system that does not contain in its loop an extended Gopinath estimator.

The Gopinath flux estimator, whose gate matrix is calculated with the (2) relations, ensures the adjustment system very good dynamic performances that gives us the possibility to assert, that such an estimator can be successfully used in industry.

In this paper we determined the upper and lower variation limits for the identified rotor resistance for which the $x_0 = b_0$ equilibrium point remains asymptotically in both the discrete and continual cases.

The following information emphasized within Table 1 for the continual case ant Table 2 for the discrete case have been obtained.

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	$M_r = M_N$	$M_r = 0$
LI	$0.6 \cdot R_r$	$0.1 \cdot R_r$
LS	$2.28 \cdot R_r$	$2.289 \cdot R_r$

Table 2	
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	$M_r = M_N$	$M_r = 0$
LI	$0.71 \cdot R_r$	$0.18 \cdot R_r$
LS	$2.272 \cdot R_r$	$2.278 \cdot R_r$

where, LI is the lower limit and LS the upper limit of variation of identified rotor resistance.

From the tables above one may notice that the upper limit for the discrete case decreases compared to the upper limit for the continual case while the lower limit for the discrete case increases compared to the lower limit of the continual case. This conclusion remains valid in both cases whet the resistant couple is either lacking or present. Also, from the tables above one may notice that the upper limit in case of lacking resistant couple increases compared to the upper limit in case of having resistant couple and the upper limit in case of lacking the resistant couple decreases compared to the lower limit in case of having resistant couple. This conclusion remains valid for both, the continual and discrete cases.

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TEACHING EMBEDDED CONTROL USING CONCURRENT JAVA

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KEYWORDS

Embedded Control, Concurrent Java, Small-scale Model Building, Remote Control.

ABSTRACT

Aalesund University College (AUC) has long and broad experience in the use of the Java Concurrency Model for process control. An important part of this work is the design and control of small-scale embedded systems. These systems include models of many kinds, such as vehicles, motion platforms, pendulums and simulated path tracking systems. The control strategies are mostly based on state space models, using modal and optimal control algorithms. Using realistic smallscale models, software and hardware capabilities and limitations can be tested for possible future full-scale industrial realizations.

INTRODUCTION

Aalesund University College (AUC) has a tradition in the design and building of small-scale embedded control systems. A vital part of the student's Bachelor program in cybernetics has been to develop and build small-scale models of many kinds of dynamic systems, such as pendulums and motion platforms and all kinds of moving vehicles. Often the starting point of a project is a commercially available model building kit, which is being technically upgraded with microcontrollers, motors, sensors and communication hardware to end up as advanced experimental test equipment. An important objective of this activity has also been to involve local industry partners in an innovative process regarding the evaluation of product ideas and potentially further product development. The choice of microcontrollers has been small RISC processors of the types Stamp and PIC. The preferred programming language has become Java, mostly due to the existence of the Java Concurrency Model (JCM) with its simple, yet extensive thread capabilities. The trend has therefore been to choose microcontrollers that have a Java runtime system and a Java Virtual Machine (JVM) included, and with development support for Java. Since 2002 the Java Community Process (JCP) has undertaken a great effort on improving the JCM model with new and improved classes in the java.util.concurrent package. Likewise in this period the Real-time Specification for Java (RTSJ) has been revised and much developed under the guidelines of the National Institute for Standardization of Technology (NIST). As a consequence of the work directed by the JCP the Real-time Java (RTJ) model is approaching the requirements of a deterministic real-time system. The development and documentation of the RTSJ standard is the responsibility of the Real-Time for Java Expert Group (RTJEG). The standard is available on the internet at the site of JCP (JCP 2005). These improvements are first being realized on Windows and Linux platforms, but are also gradually being implemented in the embedded microcontroller segment. This development of RTJ is the main argument for using Java in the control and monitoring of hardware equipment, hopefully in a successive progress towards deterministic process control with Java. Being guided by this development in RTJ the cybernetics program at AUC has gained valuable knowledge on using Java in communication and control applications. From the experimentation with small-scale models much experience has also been obtained on the possibilities and limitations of using Java for real-time applications on dedicated microcontrollers (Rekdalsbakken and Styve 2008). This paper is aimed to give a representative presentation of this kind of projects performed by students and teachers at AUC.

THE JAVA CONCURRENCY MODEL

Threads

A thread is an independent process in Java and is the central concept of the JCM. Threads run concurrently and independently within the same JVM. Threads are implemented in Java by the active object concept by inheritance from the Thread class. The thread has a run() method that executes the thread program. The central mechanism for synchronizing threads is the monitor. A monitor encapsulates a shared resource and provides a procedural interface to that resource. In Java the monitor concept relies on a *mutual exclusion* lock for each object. The monitor secures that the procedural access to the lock is executed atomically. A method or a block of code must be labelled with the synchronized modifier to activate the corresponding object's lock. The first call to the synchronized method will get the lock. Subsequent calls to synchronized procedures within that object will enter the locked state and will have to wait for the access. The methods wait() and *notify()* have opposite functions; *wait()* is used by a lock owner to temporarily release the object's lock and enter a wait state. This is usually done if a certain condition is not fulfilled. In this way access to the synchronized

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) methods of that object is again allowed. A notify() called by another thread will alert a waiting thread to regain the lock and continue execution. This thread will normally again perform the test on the vital condition. In this way *wait()* and *notify()* constitute the basic mechanism for the synchronization of threads in Java. A drawback of JCM, however, is the lack of conditional variables. These are used to discriminate between the different object locks that threads are waiting for. They will have to be implemented by the programmer. A relative time delay is implemented with the method sleep(), and the method yield() enables the current thread to give up the execution. This scheme is the basis of the JCM. By these mechanisms all common real-time devices may be implemented, like semaphores, signals, event flags, blackboards etc. The actual implementation of such methods and devices is specific for each microcontroller system. The JCM model is well documented in recent text books (Goetz 2006; Magee and Cramer 2006; Wellings 2004).

The Real-Time Specification for Java

The JCM gives an adequate platform for parallel program execution in Java. It does not, however, specifically support any real-time requirements. The RTSJ is developed on basis of the requirements on Real-time Java set by the US National Institute of Standards and Technology (NIST). RTSJ concerns the implementation requirements of the Java Virtual Machine and also gives specifications for the use of the concurrency model. The crucial property of a real-time system is determinism. In short RTSJ deals with timing requirements to the system's response to critical actions, including specifications for asynchronous event handling and transfer of control. These properties are provided as special classes in RTSJ. These mechanisms are highly dependent on the interaction between system software and the hardware. On a hardware platform supported by a traditional operating system, an application programmer often has little influence on these matters aside from following the recommendations for the use of the concurrency model. On an embedded controller system the run-time facilities are usually much simpler, but the programmer has more freedom to improvise and implement mechanisms adapted to the needs of the situation. The developing process on real-time Java and on the RTSJ standard is found at the web site of RTJ (RTJEG 2005).

Embedded Java

An increasing number of microcontrollers are supplied with an embedded JVM. On the smallest systems only a limited part of the standard Java API is available and there are also restrictions on the use of memory and the number of concurrent processes. The scheduler regimes are also usually quite simple and will vary from system to system. In this paper applications developed on two such small microcontroller systems are presented. One of these is the SBC65EC SBC card from Modtronix built around a PIC controller from Microchip Technology. This controller is furnished with a Java boot loader and a Muvium Developers Kit, including a Java runtime environment and an Integrated Development Environment (IDE). It can be programmed using standard Java, e.g. by us of NetBeans. The other system is the Javelin Stamp from Parallax Inc. Both these systems have a JVM, also called a Java OS, installed. However, both systems API software have limitations compared to standard Java SE. The Javelin has to be programmed using its own IDE. In short the Muvium system has the possibility to run concurrent threads. The scheduler is nonpreemptive, so that each thread has to voluntarily give up execution by a call to *yield()*, and the threads have no priorities. The Javelin Stamp can in principle only run a single thread. It has, however, implemented in firmware a quite extensive system of Virtual Peripherals (VP) to administer the controller's I/O functions. These VPs can either run independently in the background of the application software or in parallel in the foreground. In this way both microcontroller systems can be programmed to perform concurrent processing.

EMBEDDED REAL-TIME CONTROL

Java Microcontroller Boards

The microcontroller market offers several computer boards built upon a microprocessor with a Java interpreter integrated in hardware, or a boot loaded JVM that is tailored to the processor. In this work two microcontroller boards have been explored, the Muvium SBC65EC SBC computer and The Javelin Stamp Demo Board (JSDB). Both systems are equipped with a concurrent Java model and both have an IDE for program development and testing in Java. The benefit of working with small dedicated controllers is the close connection to hardware and hands-on control of I/O and peripherals. The drawback is the lack of or limited access to services from an OS system, but this is often outweighed by the possibilities to tailor the software to the special purpose in question. Also the IDEs for these microcontrollers have been developed to include online execution control and testing of ports and variables. Peripheral facilities have also been much enhanced on the smallest microcontrollers both for analog and digital I/O ports, often including PWM signals and ADCs of high resolution. The communication possibilities are good. quite minimum generally As а the microcontrollers support SSPI. Depending on the microcontroller board support for RS-232 and even TCP/UDP protocols, CAN and Profibus may be available.

The Muvium SBC65EC Development Board

The SBC65EC is a development board from Modtronix built around a PIC18F6627 microcontroller and with a RTL8019AS Ethernet controller and a RJ45 plug for network connection (Modtronix 2006). Muvium is the name of a JVM that can be installed on this controller with an accompanying Java API (Muvium 2005). This Muvium OS includes a simple scheduler that allows a programmer to run concurrent threads. The SBC65EC is well supplied with peripheral units, among which is a 10 Mbs Ethernet connection with a TCP/IP stack supporting socket connections for TCP and UDP. It has two serial ports with RS232 interface. The board also has 32 general user programmable I/O ports, which can be configured for instance as a 10 bits analog input and a 4 bit PWM output. The Muvium IDE on the PC uses a RS232 port for communication with the SBC65EC. The serial communication is performed by using either of the packages *Javax.com* or *RxTx*.

The Javelin Stamp Demo Board (JSDB)

The JSDB is furnished with an integrated hardware Java interpreter and an internal 16 bits bus for data transfer (Parallax 2006). This assures fast transfer of the byte code between a SRAM and the interpreter and effective execution of code. The controller is richly equipped with I/O ports and communication hardware. These peripherals are controlled by implemented firmware called Virtual Peripherals (VP). These VPs can run either in the foreground or independently in the background of the current thread. Although the runtime system allows only one running user thread at a time, the VPs supply the programmer with quite efficient tools for concurrent execution of necessary processes. The JSDB connects to a PC through a serial RS232 communication port for program download and debugging.

Small-scale Model Building

The microcontroller systems have been used in smallscale hardware models to test their capacities and abilities regarding communication and I/O functions. Many of these models are vehicles based on commercial model kits built to scale, e.g. 1:10. These model kits are modified and further developed by use of all kinds of necessary equipment, like sensors, motors and communication peripherals. The resulting models are then programmed to perform all kinds of conceivable operations, with a view to possibly later realization in industrial products. Examples are tracking systems for light sources or selected objects; automatic topological levelling for a mechanical digger, autonomous radio controlled vehicles, GPS-tracking vehicle, two-wheel balancing devices like wheelchairs, etc. Many such operations may be realistically tested by accurate smallscale models using timely equipment and methods.

TWO-WHEEL BALANCING MONSTER TRUCK

Peripherals

The aim of this project is to make a 4WD monster truck balance on its rear wheels. The car is a HPI Wheely King model, scaled 1:12 of real size. To measure the angle of the car to the vertical axis, an accelerometer of the type Memsic MXD2125G is used (Memsic 2005).

This accelerometer uses a thermal principle which also enables it to measure the angle to the vertical line, like an inclinometer. The angle is represented by a PWM signal where a pulse width of 5000 μ s represents horizontal position and a ±1250 μ s deviation from this represents ±90°. The position and velocity of the car are measured indirectly by integration and differentiation of the arc of the angle of the rear wheels. The vehicle is furnished with two 7.2 V DC motors. To control the speed of the motors a motor controller of the type Parallax HB-25 was used. This controller has a PWM output and includes an H-bridge for direction control.

Control Strategy

To be able to control the system a state space model of the car was developed (Goher and Tokhi 2008). The car is modelled as a uniform rod connected to a circular cylinder (rear wheels). The mathematics is based on physical conservation laws, i.e. Kirchoff's and Newton's laws. The derivation results in the following four-dimensional state space model:

$$\dot{z} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & \frac{K_e^2 \left(m_1 lr - J_1 - m_1 l^2 \right)}{Ar^2 R} & \frac{m_1^2 g l^2}{A} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & \frac{K_e^2 \left(Br - m_1 l \right)}{Ar^2 R} & \frac{Bm_1 g l}{A} & 0 \end{bmatrix} \cdot z + \begin{bmatrix} -\frac{K_e \left(m_1 lr - J_1 - m_1 l^2 \right)}{Ar^2 R} \\ -\frac{K_e \left(Br - m_1 l \right)}{Ar R} \end{bmatrix} \cdot u$$
(1)

where:
$$A = BJ_1 + m_1 l^2 \left(m_2 + \frac{J_2}{r^2} \right)$$
, $B = m_1 + m_2 + \frac{J_2}{r^2}$.

In these expressions the index 1 refers to the body of the truck (uniform rod) and index 2 refers to the rear wheels. The symbol K_e is the electrical motor constant, r is the radius of the rear wheels, and l is the length from the centre of rear wheels to the mass centre of the vehicle. The state variables of the system are defined as follows:

 $z_1 = x = \text{position}$, $z_2 = \dot{x} = \text{velocity}$, $z_3 = \phi = \text{vertical angle}$, $z_4 = \dot{\phi} = \text{angle velocity}$

The manipulating signal is $u = U_a$ = motor voltage. Numerical values for all constants are obtained from written specifications or through measurements. By inserting these values into model (1) a system with eigenvalues equal to $\lambda = [0 - 0.003 - 5.608 5.608]$ is obtained. As expected this reveals an unstable system.

The state-space model is the basis for controlling the physical model through the control law, $u = -\mathbf{K} \cdot \mathbf{z}$. The **K** vector may be obtained by different techniques. In this case two methods have been explored. The first is the pole placement technique using Ackermann's formula with a Butterworth polynomial forming the characteristic equation, the other is the Linear Quadric Regulator (LQR) with proper weights on the different state variables and manipulation signal. The system band width was estimated to 20 Hz and the K vector was calculated with both methods. Simulations show stable systems for both techniques, but the K values obtained by using the Butterworth polynomial became very large, and had to be scaled down. The LOR method, however, produced a control vector equal to $K = \begin{bmatrix} -44.7 & -78.9 & 6488 & 1162 \end{bmatrix}$, which resulted in the following eigenvalues for the controlled system:

$$\begin{bmatrix} -5.61+i0.22 & -5.61-i0.22 & -0.71+i0.71 & -0.71-i0.71 \end{bmatrix}$$

This shows a stable system with reasonable damping and response time. The control algorithm based on these values was simulated with good results. The regulator was then implemented in the vehicle. In such experiments much effort on trial and error has to be carried out, but eventually the vehicle was tuned to balance for shorter periods of time.

Software

The software was developed in Java with the NetBeans IDE including the Muvium library for the SBC65EC controller board. Muvium has the capability of running independent threads and includes support for common real-time mechanisms like semaphores, FIFO buffers, blackboards etc. The threads, however, have to explicitly give up execution by calling the *yield()* method. At least one thread has to extend the standard class *UVMRunnable()* to make a runnable program. A picture of the truck is shown in Figure 1, and the UML class diagram for the car software is shown in Figure 2.



Figure 1: Picture of the Balancing Truck



Figure 2: UML Class Diagram for the Balancing Truck

RADIO CONTROLLED TEST VEHICLE

Wiimote Remote Control and WiiUseJ

The objective of this project is to construct a test vehicle that can be remotely controlled from a Wiimote controller from Nintendo. Communication between the Wiimote and PC goes through a standard Bluetooth device on the PC. The incoming information is treated by use of the WiiUseJ Java library (Googlecode 2008). The information from the Wiimote over the Bluetooth connection is gathered by the PC in a data structure. These data are wrapped into a simple protocol that is being transmitted as a telegram over a TCP/IP socket connection to a Muvium controller board. The telegram contains 8 bytes, which is enough to control the remote vehicle. On the Muvium controller board the telegram is forwarded over a serial RS232 line to an onboard radio transceiver chip. The transmitted radio signals are picked up by another radio transceiver placed on a second Muvium controller board, located onboard the test vehicle. Through this communication chain the vehicle gets its control information from the Wiimote controller. The vehicle is supplied with sensors for different kinds of measurements like temperature, light and acceleration, and operates as an autonomous test vehicle sending the sensor information back to the PC. The aim is to further supply the vehicle with a camera and proximity sensors to allow for maximum independent operation, however with possible remote interference from the Wiimote controller over the radio link, see Figure 3 for an overview of the total system.



Figure 3: Circuit Diagram for Test Vehicle. Upper Part is the remote Vehicle; lower Part is the stationary PC

Socket Connection with TCP/IP

The Muvium controller board is furnished with an Ethernet connection and a Java.net program package with classes for network communication, included socket and socketService. With this package a socket connection between the PC and Muvium controller board can be set up in Java, and a TCP/IP protocol may be established. The Muvium board is furnished with a radio transceiver and functions as the remote communication link to the vehicle. On the Muvium radio transceiver a socket connection is established as a server for the PC client. On the PC a TranceiverHandler object is defined which sets up the socket connection to the Muvium board on the given IP address, and gets access to the socket's input and output streams. On the PC two independent threads are created; one is reading the data from the Wiimote controller, wrapping them into telegrams and transporting them to the Muvium radio controller over TCP/IP line. The other thread gathers the data that come in the opposite direction from the vehicle via the Muvium radio transceiver, and presents the data in a GUI on the PC.

Radio Communication

The radio communication is established by the use of a RF transceiver of the type Easy-Radio ER400TRS (LPRS 2003). It has a frequency of 433MHz and 10 mW output power. This gives a range of 250 metres in an area with free sight. To improve the range an extra antenna was mounted. The interface is via a half-duplex serial RS232 line.

Sensors

The test vehicle is supplied with several kinds of sensors to monitor its operations and to explore the possibilities for use in practical situations. The main sensors are a Memsic MXD2125G thermal 2-axes accelerometer, and a Phillips KTY81-120 resistance temperature sensor. In addition the battery supply voltage is measured by an analog input port on the Muvium controller, and the radio signal power is read from the transceiver. The accelerometer is used to measure extreme stress situations on the vehicle, e.g. a crash or tip over.

Software

All the software is written in Java using NetBeans IDE. On the PC the WiiUseJ library is used for communicating with the Wiimote remote controller, including the *WiimoteListener* used to capture events from the Wiimote controller. A user-friendly GUI was developed by use of the Java interface *KeyListener*, which enables events to be generated when using the keyboard or the mouse. The SBC65EC controller boards are programmed using the Muvium API delivered with them. On the test vehicle three independent threads are created in the *main* class to run on the controller. These threads have the following responsibilities: *DatagramHandler* – receive and control the telegrams from the radio transceiver. Effectuate the commands contained in the telegrams.

SendResponseThread – collect the information obtained by the onboard sensors and retransmit the data to the PC in a proper telegram.

SafetyThread – by use of the accelerometer, monitor the motion of the car and stop its operation if a hazardous condition occurs (e.g. a car crash). A message is sent to the host PC.

These threads use methods in auxiliary classes to effectuate the necessary operations on the car peripherals.

GPS TRACKING VEHICLE

Remote or Autonomous Control

This vehicle is designed as an autonomous path tracking device controlled by a JSDB board and guided by an embedded GPS receiver. The vehicle, however, is also connected to a remote PC through a radio connection. Thus the vehicle can by manually controlled from the PC by a Wiimote controller, or it can follow a predestined path by use of the GPS coordinate information. The radio transceiver is of the type Easy-Radio ER400TRS as described above.

GPS Tracking

The vehicle is furnished with a GlobalSat GPS EM406A receiver (GlobalSat 2007). This is an OEM module with SiRF Star II chipset including an antenna. It communicates on a 4800 baud serial line supporting the NMEA 0183 protocol. It has high tracking sensitivity and a position accuracy of up to 5 metres. The acquisition time is 0.1 sec in average. The GPS is connected to the Javelin stamp's serial RS232 interface, which runs independently as a VP in the background. In the calculations of the car position a starting origo point is defined. On 62° N the ratio of 1° latitude to 1° longitude is 2.16. In the GPS coordinate measurements this ratio is counted for, and the arc tangent function is used to calculate the angle to the next waypoint. In this way the car is following a path by linear extrapolation from waypoint to waypoint. This is not a very precise method because errors in position will accumulate, and therefore a new correct origo has to be determined after some steps. Future improvements in GPS accuracy may give opportunity for a continuous path update towards the waypoint.

Motor Control

Motor control is performed with a Pololu Micro Serial Servo controller (Pololu 2005). This module controls up to eight servo motors through PWM output ports. It connects by TTL logic serial lines (SSPI) both to the JSDB board and to the ER400TRS radio transceiver. In this way the speed and steering of the car may be controlled either from the Javelin stamp onboard the car or from the Wiimote controller on the PC through the radio communication line. Figure 4 shows the circuit diagram for the connection between the radio transceiver and the Pololu controller, and Figure 5 shows the connection diagram between the PC and the radio transceiver.



Circuit Diagram for the Connection of ER400TRS and the Pololu Micro Serial Controller



Figure 5 Circuit Diagram for the Connection of the PC and ER400TRS

Software

In this project the software for the autonomous GPStracking function is developed in Java for the Javelin stamp processor using the dedicated Javelin IDE and Java libraries. The serial connections from the Javelin stamp to the GPS and Pololu circuits are realized by use of the UART and SSPI VPs on the Javelin. These programs are performing their tasks independently of the main thread. In addition the software consists of an independent Java program running on the PC for the radio controlled steering of the car. This program uses the WiiUseJ library, implementing the WiimoteListener to capture events from the Wiimote remote controller. It also uses the (now obsolete) javax.com package for serial communication to the radio transceiver. The *javax.com* may be substituted by another serial communication package, e. g. RxTx.

RESULTS

These student's projects have revealed that Java is a program language that may be successfully used for process control applications on embedded systems. The great ongoing activity on the development of the JCM model and not least on the RTSJ standard encourages real-time programming with Java. Java is seen to have the necessary real-time mechanisms and also the power for fulfilling the timing requirements in process control. There is, however, still a way to go to guarantee determinism with the JCM. This is a general design problem, and much can be done by building specifically tailored dedicated systems.

CONCLUSION

The model building activity has two main goals; to explore the possibilities and limitations of using Java as a real-time system in embedded process control, and to create a context for experimenting with dedicated microcontrollers and the existing assortment of peripheral circuits in realistic process control and communication applications. The small-scale models have given a context for the testing of communication equipment and software, and the tools for experimenting with different kinds of control algorithms. This experience will improve the understanding of communication and control systems in general, and may give ideas for the building of full-scale devices. The students get a practical approach to control systems and the possibility to test the theories they learn in cybernetics and real-time programming. Finally, the scientific staff is inspired to further explore this technology into new student projects for future challenges. Some of these models may also give offspring into new products in collaboration with local industry partners.

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NUMERICAL MODELING AND EXPERIMENTAL RESULTS OF HIGH CURRENTS DISMOUNTABLE CONTACTS

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ABSTRACT

The paper presents an electro-thermal numerical model which can be used for the modelling and optimization of high currents dismountable contacts for dc current. The model is obtained by coupling of the electrokinetic field problem with the thermal field problem. The coupling is carried out by the source term of the differential equation which describes the thermal field. The model allows the calculation of the space distribution of the electric quantities (electric potential, the gradient of potential and the current density) and of the thermal quantities (the temperature, the temperature gradient, the Joule losses and heat flow). A heating larger than that of the current lead appears in the contact zone, caused by the contact resistance. The additional heating, caused by the contact resistance, is simulated by an additional source injected on the surface of contact. Using the model, one can determine the optimal geometry of dismountable contact for an imposed limiting value of the temperature

INTRODUCTION

The optimization of the dismountable contacts (Figure 1) for high currents (500 - 4000 A), used in the design of electrical equipment in metal envelope, is possible by solving a coupled electrical and thermal problem. The dismountable contact of a system of bus bars has a non-uniform distribution of current density (Figure 2) on the cross-section of the current leads. The non-uniform distribution of the current density implies a non-uniform distribution of source term in the thermal conduction equation.

The distribution of the electric quantities can be obtained by solving of Laplace equation for electric potential. The solution of this equation depends on the temperature through electric conductivity. In its turn the electric conductivity influences the source term in the thermal conduction equation and thus the value and the distribution of the temperature of electrical contact. Dan FLORICAU POLITEHNICA University of Bucharest Faculty of Electrical Engineering E-mail: df@conv.pub.ro Serghie VLASE Research Insitute ICMET, Craiova, Romania Electrical Apparatus Laboratory E-mail: vlase_serghie@yahoo.com



Figure 1: Typical Dismountable Contacts



Figure 2: Current density distribution

Obtaining the correct distributions for the electric quantities (potential, intensity of the electric field, current density and losses by Joule effect) and thermic (the temperature, the gradient of temperature, density of the heat flow, the convection flow on the contact surface, etc) is possible by the coupling of the two problems, electric and thermal. The numerical model allows the calculation of the constriction resistance (caused by the variation of the cross section of the current lead).

MATHEMATICAL MODEL

The mathematical model used for obtaining the numerical model has two components, the electrical model and the thermal model, coupled by the electric conductivity, which varies according to the temperature, and the source term.

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Electrical Model

The electrical model is governed by a 2D model described by the Laplace equation for the electric potential

$$\frac{\partial}{\partial x} \left(\sigma(T) \frac{\partial V}{\partial x} \right) + \frac{\partial}{\partial y} \left(\sigma(T) \frac{\partial V}{\partial y} \right) = 0 \qquad (1)$$

where electric conductivity and thus the electrical resistance vary according to the temperature as

$$\rho(T) = \rho_{20} \left(1 + \alpha_R (T - 20) \right)$$
(2)

Knowing the electric potential, one can obtain the intensity of the electric field $\vec{E} = -\text{grad }V$ and the current density $\vec{J} = \sigma \vec{E}$ (law of electric conduction). The Joule losses (by the unit of volume) which represents the source term in the thermal conduction equation are calculated by the following relation

$$S(T) = \vec{J} \cdot \vec{E} = \rho(T)J^2 = \sigma(T)E^2.$$
(3)

Thermal Model

The thermal model is governed by the thermal conduction equation in steady state

$$\frac{\partial}{\partial x} \left(\lambda(T) \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda(T) \frac{\partial T}{\partial y} \right) + S = 0 \quad (4)$$

where λ - the thermal conductivity which is considered constant in the temperature range of the current lead (bellow 200 °C).

DOMAIN OF ANALYSIS AND BOUNDARY CONDITIONS

One considers a simplified analysis domain which is presented in Figure 3 and Figure 4 where one neglects the existence of the fastening bolts.

The boundary conditions of the electrical model are presented in Figure 3. In the general case, one knows the current I carrying the current lead and which determines a voltage drop $V_1 - V_2$. In this model, one initializes a voltage drop for which one calculates the current which corresponds to it (at each iteration) and then in a iteration loop one modifies the voltage drop to obtain the desired value of the current.

The current which passes any section of the current lead is calculated by the following relation

$$I = \int_{S} (\vec{J} \cdot \vec{n}) \mathrm{d}S \tag{5}$$

where \vec{n} - the normal at S which is the cross-section of the current lead.

The two assembled bars are considered sufficiently long

to set, on the boundaries AB and CD (Figure 4) the boundary conditions of Neumann homogeneous type. If the length of segments AE and FD (375 mm) of Figure 4 is long enough the temperature distribution is uniform and consequently the temperature gradient is almost zero and the axial thermal flow is also zero.

On the other borders, one sets boundary conditions of the convection type, with a global heat exchange coefficient h (by convection and radiation, $h = 14.5 \text{ Wm}^{-2} \text{ K}^{-1}$, increased by a coefficient that takes into acount the heat transfer through the side surfaces) to the environment having the temperature T_{∞} (Popa et al. 2006a).



Figure 3: Analysis Domain and Boundary Conditions for Electrical Model.



Figure 4: Analysis Domain and Boundary Conditions for Thermal Model (AE = FD = 0.375 m, EF = 0.1 m).

NUMERICAL ALGORITHM

The numerical model is obtained by the discretization of the differential equations (1) and (4) by using the finite volumes method (Popa 2002). The coupled model is of alternate type (Meunier 2002) where the equations are solved separately and coupling is realized by the transfer of the data of one problem to the other. The two problems (electric and thermal) are integrated in the same source code and thus use the same mesh. The numerical algorithm is shown in Figure 5. The criterion of convergence of the coupled model was selected the value of the current, through the current lead, calculated using the relation (5). One used a mesh having 3787 nodes (with $\Delta x = \Delta y = 1.66$ mm). The imposed percent relative error, for electrical and thermal models, was 10^{-7} and for coupled model was 10^{-5} . The convergence of the coupled model is very fast $(4 \div 6)$

iterations). If the error is reduced then the number of iterations increases but this is not necessary. The desired value of the current in contact is adjusted by varying the voltage drop on contact. The number of iterations for the electrical and thermal models decreases sharply with the stabilization of current.

The numerical validation of the model was made using a simplified analysis domain with a current lead with variable cross-section (Popa et al. 2006a), (Popa et al. 2006b). The numerical validation of the results of this simplified model was made by using the software QuickField Professional for the electrical and thermal models. One can see a very good agreement between our results and the results obtained using the QuickField software.



Figure 5: Simplified Diagram of Numerical Algorithm.

NUMERICAL RESULTS AND EXPERIMENTAL VALIDATION

The Figures 6, 7, 8, 9 and 10 present some numerical results. The dimensions of the analysis domain are those of Figure 4. The principal difficulty, in modelling and the temperature simulation distribution of а dismountable contact, is to take into account the resistance of contact (especially disturbance resistance). The contact resistance model is presented in the next paragraph. The optimization of the contact design supposes to determine the value of dimension l_c such that the maximum temperature, in the contact region, remains lower than the acceptable limiting value allowed by standards.

For the case presented ($l_c = 100 \text{ mm}$ and I = 620 A) the calculated losses by Joule effect with constriction resistance are 28.89 W, while calculated Joule losses without constriction resistance are 24.91 W. Varying overlapping length of the bars l_c (see Figure 1) the maximum contact temperature has a linear dependence with l_c (Popa et al. 2006b).



Figure 6: Potential Distribution in the Contact Region (in mV).



Figure 7: Electrical Field Distribution in the Contact Region (in V/m).



Figure 8: Current Density Distribution in the Contact Region (in A/mm²).



Figure 9: Temperature Distribution in the Contact Region (in °C).



Figure 10: Gradient of Temperature in the Contact Region (in ° C).

The experimental model and the measuring points are presented in Figure 11 (the measuring points are placed in the center of surface). The values measured in these points, using a digital thermometer with contact (Fluke 54 II) are shown in Table 1. The numerical results for the thermal field, illustrated in Figure 9, compared with the experimental results (see Table 1) show a good agreement. For exemple the error in the measurement point T_4 (in the center of the contact) is 2.13 %. The experimental data of Table 1 were measured for a tightening force of screws of 50 N.



Figure 11: Points of Temperature Measurement.

Table 1: Experimental Results

Point	T_1	T ₂	T ₃	T_4	T ₅	T ₆	T ₇
T [°C]	29.3	29.3	29.4	29.8	29.4	29.3	29.3

For the considered contact geometry and the current of I = 620 A, the voltage drop measured between the limits *AB* and *CD* (see Figure 4) was 11.98 mV, while the voltage drop controled to get the current imposed in the numerical model was 11.2 mV.

The experimental results of Table 1 were obtained for the ambient temperature of 20.5 °C.

Figure 12 shows the thermal image of the contact zone obtained with the thermal camera. One can observe the scews areas which is colder. The scews help to cool the contact region by enlarging the surface of thermal eschange with surrouding environment.



Figure 12: Thermal Image of the Contact Region

CONTACT RESISTANCE MODEL

The source term determined by the contact resistance is calculated by the following relation

$$S_c = \frac{R_c I^2}{(nc-1)\Delta x \Delta y H},$$
(6)

where Δx and Δy - the dimensions of the control volume, nc - the number of mesh points in the contact region (see Figure 13), H - the bus bar width (see Figure 1).

The contact resistance R_c is calculated with the following relation (Hortopan 1993)

$$R_{c} = \frac{\rho}{\pi a n} \arctan \frac{\sqrt{d^{2} - a^{2}}}{a} - 1.2 \frac{\rho \sqrt{d^{2} - a^{2}}}{A_{a}} + \frac{R_{ss}}{n \pi a^{2}}$$
(7)

where ρ - the electric resistivity, *n* - the number of contact points, A_a - the total area of contact (see Figure 14) and R_{ss} - the specific resistance of oxide film of contact point (in Ωm^2).



Figure 13: The Mesh in Contact Region

The radius of contact surface a is calculated from Holm's relation (Hortopan 1993)

$$a = \sqrt{\frac{F}{\pi n \xi H_d}}.$$
(8)

where F - the tightening force, ξ - Prandtl coefficient,

 H_d - material durity.



Figure 14: Physical Model of Contact Region

The relation (7) does not take into account the variation of contact resistance with temperature. To take it into account one can use the relation (Hortopan 1993)

$$R_{c}(T) = R_{c}(20) \left(1 + \frac{2}{3} \alpha_{R}(T - 20) \right)$$
(9)

where α_R - the variation coefficient of electric resistivity with temperature, $R_c(20)$ - the contact resistance at 20 °C.

The contact resistance model was implemented in numerical model of dismountable contact. For a constant value of the current (I = 620 A), varying the tightening force of the screws one can get the variation of the maximum temperature versus tightening force.

CONCLUSIONS

The created model can be used for the optimization of the current leads of high currents with variable crosssection, such as the dismountable contacts. The model allows the calculation of the constriction resistance of current lead, the constriction resistance of contact region and takes into account the specific resistance of oxide film of contact point which is an important component of the contact resistance.

Numerical model created allows evaluation of the maximum temperature in the contact area as a function of the tightening force of the dismountable contact.

An improvement of the model is possible taking into account the presence of the tightening screws and usage of the model of contact resistance moore precise as exemple the model given by Greenwood (Feng et al. 1998). The model is valid only for dc. In alternating current Equation (1) must be replaced by a magnetodynamic equation.

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CONTROLLED SWITCHING – SOLUTION FOR REDUCING THE OVERVOLTAGES AT COMMUTATION OF THE TRANSPORT AND DISTRIBUTION LINES

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KEYWORDS

Controlled switch, distributed parameter line, model.

ABSTRACT

Recently, worldwide, the controlled switch became a technical solution for reducing the switching stress. After 90es, the number of equipment which uses the controlled switch fast increased, mainly due to the achieved performances.

The controlled switching can be applied to any type of commutations. Now there are dedicated controllers which are used more often for the switching of the transport and distribution lines, of the small inductive loads, of the capacitors batteries, or the energizing the no load power transformers. The paper deals with the simulation of the commutation of a transportation line by using the distributed parameters model. The controlled switch of the line is compared with the uncontrolled one, highlighting the major differences in what concerns the stress.

TRANSPORT AND DISTRIBUTION LINES SWITCH

When the long lines are energized, undesired over voltages can be generated in the transport and distribution networks. These are caused by the propagation, reflection and refractions of electromagnetic waves, both in ramifications points and end of the lines. Such phenomenon both occur when the lines are quick re-energized after a disconnection. The cause of the over voltages in this case are the residual charges on the line. As will be seen, both the over voltages and their slopes determine important stress of the equipment insulation.

When connected, at the end of the long lines over voltages can occur due to more causes. For lines shorter than 1500 km, the input impedance has capacitive character and the voltage drop on the equivalent inductive reactance of the system has the same sign with the supplying fem. Consequently, this voltage drop is added to the fem. Thus, the resulted overvoltage highly depends by the line length and by the short circuit power of the system.

Another cause of the over voltages resides in the oscillations which occur when the initial repartition of the voltage across the line is replaced by the new repartition corresponding to the new steady state operation, after its connection.

The stress of the insulation depends both by the amplitude of the overvoltage and by its shape, characterized by two parameters: rising duration and falling duration. (Gusa 2002).

The mathematical models used to determine the over voltages can be more or less complex, depending on the characteristics of the studied commutation phenomenon. The long lines can be modeled by circuits with either uniform distributed parameters or concentrated parameters. The models can be single phase or three phase ones.

The over voltages when a line is energized can be analytically estimated if two hypotheses are considered: the lines have no losses and all the three phases of the breaker are simultaneously connected.

For the analytically evaluation of the over voltages at the line energizing with no residual charge on the line, the simplified diagram in Figure 1 can be considered.

The equation specific to the equivalent electric system is.

$$e_s = u_1 + L_s \cdot \frac{di_1}{dt} \,. \tag{1}$$

The equations specific to the uniform distributed long line model are:

$$-\frac{\partial u}{\partial x} = r \cdot i + L \cdot \frac{\partial i}{\partial t}, \qquad (2)$$

$$-\frac{\partial i}{\partial x} = g \cdot u + C \cdot \frac{\partial u}{\partial t}, \qquad (3)$$

where:

- $\cdot e_s$ the instantaneous value of the fem of the system;
- $\cdot u_1$ instantaneous voltage at the front end of the long line:

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Figure 1: Simplified Equivalent Diagram of a No Load Line when is Connected

- $\cdot i_1$ the instantaneous value of the current at the front end of the long line;
- $\cdot L_s$ the inductance of the supplying electric system;
- \cdot *u*, *i* the voltage and the current in a point of the line;
- \cdot r, L, g, C the parameters of the line per length unit.

By solving the equations (1-3), the voltage at the end of the line results:

$$u_{2}(t) = B \cdot \sin(\omega t + \alpha) - -\sum_{k=1}^{n} B_{k} \cdot \cos\left(\omega_{k}t - \operatorname{arctg}\left(\frac{\omega}{\omega_{k}} \cdot \operatorname{ctg}\alpha\right)\right), \quad (4)$$

where

 ω_k are the roots of the equation (5)

$$\operatorname{ctg} \tau \omega_{k} = \frac{L_{s} \cdot \omega_{k}}{Z_{c}}, \qquad (5)$$

$$B = \frac{E_{m}}{\cos \tau \omega - \frac{L_{s} \cdot \omega}{Z_{c}} \cdot \sin \tau \omega}, \qquad (5)$$

$$B_{k} = E_{m} \cdot \frac{\omega_{k}^{2}}{\omega_{k}^{2} - \omega^{2}} \cdot \frac{1}{\cos \tau \omega_{k} + \frac{\tau \omega_{k}}{\sin \tau \omega_{k}}}, \qquad (5)$$

 $\boldsymbol{\alpha}$ is the phase of the source voltage at the connection instant.

For the front end of the line results the following expression of the voltage

$$u_{1}(t) = B \cdot \sin(\omega t + \alpha) \cdot \cos \omega \tau - -\sum_{k=1}^{\infty} B_{k} \cdot \cos \omega_{k} \tau \cdot \cos \left(\omega_{k} t - \operatorname{arctg} \left(\frac{\omega}{\omega_{k}} \cdot \operatorname{ctg} \alpha \right) \right)^{\frac{1}{2}}$$

B and B_k being the same as in (4).

The obtained expressions of the voltages at the front end and at the end of the long lines show that the maximum overvoltage factor at the end of the line is greater than 2 and also greater than the factor at the front end of the lines.

The over voltages can be reduced by using breaker with pre-insertion resistance or by using variable resistance dischargers.

An intelligent method for avoiding the over voltages when transport and distribution lines are re-energized is the using of the controlled switch. The method is based on the control of the difference between the source voltage and the residual voltage on the line. The reclosing command is supplied at the instant when this difference is minim. In this case, the over voltages will have the same values as when the line with no residual charge is connected. The breaker must have the facility to control independently each pole. This is the case studied further.

MATLAB SIMULINK MODEL FOR CONTROLED SWITCH OF THE TRANSPORT AND DISTRIBUTION LINES

The model of the distributed parameters long line was the one available in the SimPowerSystems of Matlab.

The Distributed Parameter Line block implements an Nphase distributed parameter line model with lumped losses. The model is based on the Bergeron's traveling wave method used by the Electromagnetic Transient Program (EMTP) (Dommel 1969).

In this model, the lossless distributed *RLC* line is characterized by two values (for a single-phase line): the

surge impedance $Z_c = \sqrt{\frac{L}{C}}$ and the phase velocity

 $v = \sqrt{\frac{C}{L}}$. The model uses the fact that the quantity u+Zi

(where *u* is line voltage and *i* is line current) entering one end of the line must arrive unchanged at the other end after a transport delay of $\tau = l/v$, where *l* is the line length. By using the current injection method of SimPowerSystems, a two-port model was derived.

For multiphase line models, modal transformation is used to convert line quantities from phase values (line currents and voltages) into modal values independent of each other. The previous calculations are made in the modal domain before being converted back to phase values. In comparison to the PI section line model, the distributed line represents wave propagation phenomena and line end reflections with much better accuracy.

The Simulink model of the simulated lines is the one depicted in Figure 2.

For comparison, two identical lines were considered, one switched uncontrolled and the other with control of the re-closing instant. Each of them is switched by a breaker. For both of them, the moment of the opening is the first zero crossing of the current after the opening command was applied. The uncontrolled breaker is reclosed at a given time. The re-closing occurs instantaneously.



Figure 2: The Simulink Model for the Two Types of Switching

The breaker corresponding to the controlled switch line is reclosed by controlling the difference between the source voltage and the residual voltage on the line. Its reclosing command, given arbitrarily, is validated and applied only at the first instant when this difference is minim. The dialog boxes of the two breakers are depicted in Figure 3.

Block Parameters: Breaker 2 uncontrolled	? 🗙	
Breaker (mask) (link) Implements a circuit breaker with internal resistance Ron (Ron, required by m cannot be set to zero). First mput [1] and output [2] are the two breaker terminals. 2nd input [c] is a 5 logical signal controlling the breaker. When, 2nd input becomes greater than	odel , Simulink n zero the	
breaker closes in tanktoneously. When 2nd input becomes zero, the breaker the next ourent zero-crossing. Parameters Breaker resistance Ron (0hm): [0 1 Initial state (0 for 'open', 1 for 'closed'): [1 Snubber resistance Rs (0hms): [init Snubber capacitance Cs (F): [0 Switching times (c): [0 Sample time of the internal timer Ts(s): [0 External control of switching times Measurements None	opens at	a)
QK Cancel Help	Apply	
<u>QK</u> <u>Cancel</u> <u>Help</u> Block Parameters: Breaker 1: external control Breaker (mask) [link] Inglements a circuib breaker with internal resistance Ron (Ron, required by m cannot be set to zero). First input (1) and output (2) are the two breaker terminals. 2nd input (c) is a a logical signal controlling the breaker. When 2nd input becomes greater tha breaker closes instantaneous). When 2nd input becomes greater the the next current zero-crossing. Parameters Breaker resistance Ron (Dhm):	Apply	
DK Eancel Help Block Parameters: Breaker 1: external control Breaker (mask) (link) Implements a circuit breaker with internal resistance Ron (Ron, required by m cannot be set to zero) Frist post [1] and output [2] set the two breaker terminals. 2nd input [o] is a 1 logical signal controlling the breaker. When 2nd input becomes greater the breaker closer instantaneously. When 2nd input becomes greater the breaker resistance Ron (Dhm): Parameters Breaker resistance Ron (Dhm): [0,1] Initial state [0 for 'open', 1 for 'closed']: [n' Snubber resistance Rs (Dhms): [n' [n' [Staten al control of switching times Measurements	Apply codel , Simulink n zero the opens at	b

Figure 3: The Dialog Boxes of the Uncontrolled Switch (a) and of the Controlled one (b)

The simulation was run for a long line having the following parameters:

- \cdot length = 200 km;
- · resistance per unit length $R = 0.0339 \Omega$ /km;
- inductance per unit length $L = 1.04 \cdot 10^{-3}$ H/km;
- · capacitance per unit length $C = 1.089 \cdot 10^{-8}$ F/km;
- \cdot supplying voltage = 220 kV.

For controlling the re-connection instant, a Simulink block *Switch control* was created which issues the external command for Breaker 1 (Ivanov 2007). This block, Figure 4, monitors the absolute value of the difference between the supplying voltage and the voltage at the end of the line. When this difference is minimum (detects the tendency to increase), the external command is validated and delivered as output to the breaker, which at its turn, switch on instantaneously.

The command for opening the breaker is not synchronized with the circuit state. The breaker opens at the first zero crossing of the current after the turn-off command.



Figure 4: The Switch Control Block

By the dialog box of the block, Figure 5, the disconnection and re-connection instants can be specified. The reconnection itself occurs at the first minimum of the difference between the supplying voltage and the voltage at the end of the line, after the reconnection time specified in the dialog box.

Block Parameters: Switch control
Switch control (mask)
Validates the re-closing instant when the difference beteween the source voltage and the voltage at the end of a long line is minimum.
Parameters
Disconnection time [s]
0.02
Reconnection time (will wait for minimum) [s]
0.075
<u>D</u> K <u>C</u> ancel <u>H</u> elp <u>Apply</u>

Figure 5: The Dialog Box of the Switch Control Block

SIMULATIONS RESULTS

The simulation of the reconnection of the two lines (uncontrolled – Line 2 and controlled one – Line 1) was performed for similar conditions: disconnection command at 0.02s and reconnection command at 0.075s. The disconnection of the both lines occurs at the first zero crossing of the current after the command instant (0.025s as can be seen in Figure 6).



Figure 6: The Currents in the Two Lines

The reconnection is instantaneously for the Breaker 2 (uncontrolled) when the command is issued (0.075 s). The reclosing of the controlled breaker is delayed until the minimum of the difference between the supplying voltage and the voltage at the end of the line occurs (Figure 7).



Figure 7: Reconnection instants

As can be seen both in Figure 8 and the detail from Figure 7, the overvoltage at the end of the uncontrolled line is quite important (overvoltage factor 2.73). On the controlled switch line the overvoltage is almost null, the voltage at the end of the line being practically identical with the supplying voltage (Figure 7).



Figure 8: Voltages at the end of the lines after reconnection

The processes at the reconnection determine high stress of the insulation. In Figure 9 is plotted the slope of the voltage at the end of the two lines. As can be seen, the stress of the uncontrolled line reaches more than $12,000V/\mu s$. For the controlled switch line the stress is almost absent, as can be seen in the detail plotted in Figure 10.



Figure 9: The slope of the voltage at the end of the reconnected lines



Figure 10: Detail of the slope of the voltage at the end of the reconnected lines

CONCLUSIONS

The paper analyzed the stress which occurs at the reconnection of the long lines. If no measures are carried out, the overvoltage and the corresponding voltage slope at the end of the line rich dangerous values.

If the switch-on process is controlled and synchronized with the minimum of the difference between the supplying voltage and the voltage at the end of the line, the additional stress is almost inexistent. Such control must be performed on each pole of the breaker.

In practice, the control of the reconnection must take into account the delay introduced by the beaker actuation mechanism, specific for each type of mechanism. This delay is at its turn, dependent on the pause time after the last actuation, on the ambient temperature and on the total number of actuation maneuvers done during the life time.

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USING CO-SIMULATIONS IN FAULT TOLERANT MACHINE'S STUDY

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KEYWORDS

Fault tolerant electrical machines, switched reluctance machines, co-simulation, numerical field computation.

ABSTRACT

The Switched Reluctance Machine (SRM) is ideal for safety critical applications (aerospace, automotive, defense, medical, etc.) where it is desirable that the electrical drive system to be fault tolerant. During the design of a fault tolerant electrical drive system it is indispensable to use advanced simulation techniques. Finite elements method (FEM) based magnetic field computation programs are the most precise tools in simulating the electrical machines. These programs must be embedded in a general simulation platform.

The paper deals with the analysis of a proposed SRM's fault tolerant capacity. The study was performed by means of a coupled simulation program. The main program was built up in Simulink[®], the most widely used dynamic system simulating platform. The SRM was modeled using the Flux 2D FEM based numerical field computation program. The machine's model was connected to the main program thru the Flux-to-Simulink link.

This co-simulation technique proved to be a very useful tool in the fault tolerance study of the proposed SRM.

INTRODUCTION

When designing a new technical system the flowchart given in Fig. 1 must be followed (Lewis 1974).



Figure 1: Design flowchart

The design is created firstly in the mind of the engineer. Later a list of specifications must be identified including

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) with the envisions which would satisfy the design's requirements. In the next stage the designer creates (firstly in his own mind) a product that meets the specifications. Next the "mind model" of the new product must be transferred into a "symbolic" or "physical" model.

It is usually best to work with symbolic models at first, because they are less expensive than physical (laboratory) models. A symbolic model is a mathematical model of the system which describes its basic behavior.

By simulations (practically by solving the equations of the mathematical model) the entire behavior of the system can be studied, and important conclusions can be drawn on the way the designed system fulfills the requirements. Based on these conclusions modifications in the design have to be performed. This checking loop should be completed until the system is closed to that required.

Only in this stage of the design an experimental model of the system is worth to be built up. If both the results obtained via simulations and experiments are acceptable the prototype of the system can be built up and tested. The final decision on the correctness of the design shall be stated only based on the test results.

Upon these is clear how important the modeling and simulations are.

FAULT TOLERANT ELECTRICAL DRIVE SYSTEMS

The *fault tolerance* by definition is a basic characteristic of a system that ensures its continuous function even after a fault occurs, that would cause a normal similar system to malfunction (Blanke 2006).

The fault tolerant concept emerged for the first time in information technology (IT). It meant an increased level of continuous operation of computer equipment. Later more and more fault tolerant equipments were connected together in order to form a fault tolerant system (Isermann 2005). The result was an operational unit having certain fault tolerant level, as a sum of the safety levels of each equipment of the system.

A system is *reliable* when it is capable of operating without material error, fault or failure during a specified period in a specified environment. From another point of view a system is *dependable* if it is available, reliable, safe, and secure (Laprie 1992).

The fault tolerant design of complex electrical systems is becoming our days a necessity for a growing number of fields, far beyond its traditional application areas, like aerospace, military and vehicles.

For example a fault of an electric drive system used in propulsion applications can be critical, since an uncontrolled output torque may have an adverse impact on the vehicle stability, which ultimately can risk the passenger safety. A failure of an electrical drive system can have disastrous effects also on a plant's ability to function. Both the converter and motor faults can cause unscheduled downtimes that can result in lost production and revenue (Ruba 2008a and Suresh 2006).

These and similar applications stimulated the researches in the field of fault tolerant electrical machines and drives (Rene 1992).

In safety critical applications both the electrical machine and its power converter must be fault-tolerant.

In the last decade several proposals to improve the electrical machine's reliability had been published. The fault-tolerant machine must have a special design. Inherently by increasing the machine's fault tolerance its losses could be greater and its efficiency less than those of its usual counterpart (Ivonne 2008).

Thanks also to the improvements in the field of power electronics and of digital signal processing today intelligent solutions can be provided in designing a fault tolerant electrical drive system.

The separate phase feeding and control of the machines are the most frequently used methods to achieve the required fault tolerant capacity (Heimerdinger 1992 and Zhang 2003).

THE PROPOSED FAULT TOLERANT SWITCHED RELUCTANCE MACHINE

The SRM in study having a 12/14 pole structure is shown in Fig. 3 (Ruba 2008c). This structure emerged from the classical 12/8 model (Krishnan 2001), as that could be transformed relatively easily in a fault tolerant variant.



Figure 3: The proposed fault tolerant SRM

The proposed modifications were implying both the rotor structure (Ruba 2008b) and the connection of the stator windings.

The winding scheme is a six phase duplex type. Practically each phase is split into two channels. At each time two channels, diametrically disposed, are fed (see Fig. 2). Hence at each moment two pairs of adjacent stator poles are contributing to the torque development. In case of a fault on one channel this will not contribute anymore to the torque generation. The second channel connected in parallel is independent of the faulty one and will continue its operation. This winding connection helps the motor to overrun the poles with faulty phases and to minimize the torque ripple.

As it can be seen in Fig. 2 the proposed SRM has shorter flux paths as its classical counterpart, which means less iron losses.



Figure 2: The flux lines in the SRM

The machine is fed from a special power converter (see Fig. 4), which has a separate half H-bridge circuit for every channel in order to be able to control each one independently, as requested by the fault tolerant design.



Figure 4: The converter of the proposed SRM

A main disadvantage of the proposed 12/14 fault tolerant SRM is its power converter (Szabó, 2008). This

to be also fault tolerant has to be complex, and able to detect and isolate the defects. It has 24 power switches and 24 reverse current diodes. The separate command of each channel will increase its costs.

THE COUPLED SIMULATION PROGRAM

Modeling complex electromechanical systems is a rather difficult task, because such systems often have sub-systems, components and aspects whose structure, as well as behavior cannot be described in a single comprehensive formalism. Different approaches to model such complex systems are possible (Vangheluwe 2002):

- i.) A single super-formalism may be constructed which subsumes all the formalisms needed in the system description.
- ii.) Each system component may be modeled using the most suitable formalism and tool. To investigate the overall behavior of the system, co-simulation can be used. In this approach, each component model is simulated with a formalism-specific simulator. In this case the co-simulation engine orchestrates the flow of input/output data in a data-flow fashion.

In order to analyze the fault tolerance of the proposed SRM adequate simulation programs are required. Hence, the electrical machine and its electronic converter must be simulated by means of coupling two software packages.

The MATLAB/Simulink[®] environment is perfectly suited for the platform that simulates the converter and imposes the different working regimes and machine conditions. Flux 2D solve numeric field computation problems, like modeling electrical machine structures. By coupling these two platforms, simulations suitable for in depth analysis can be accomplished.

It should be mentioned that the co-simulation term has also other meanings. It is also used for the joint simulation of the hardware and the software. In this case the co-simulation is usually applied to substantiate heterogeneous specifications, or to validate the hardware and software parts of a complex electrical system and their interactions (Ruelland 2001). In other cases this term covers the association of a numerical (digital) and continuous models of a complex system (Belhadj 2003).

Firstly the machine's geometry was built up using the graphical commands of Flux 2D. Also in this pre-processing stage the materials were assigned to each subdomains (stator and rotor iron core, windings, etc.).

Next the mesh required by the FEM was generated. This is an essential stage hence both the precision and the computation times depend on the correct generation of the mesh. It must be dense enough for precise calculation and also optimal for not consuming a lot of the computational time (Hameyer 1999). The most attention was paid to the mesh round the air-gap, the most important part of an electrical machine. In the next step the electrical circuit attached to the machine's model was set up. The proposed 12/14 SRM structure has 6 phases, each split into 2 channels. The electrical circuit for a single channel of the machine in study is given in Fig. 5.



Figure 5: Electric circuit of one channel

The circuit follows the arrangement of a classical H-bridge topology. The power switches are replaced by resistors. These resistors can be easily controlled from outside the circuit. For the ON / OFF states of the power switches a low (0.004 Ω), respectively a high value (100 k Ω) for the resistance is imposed.

Usual coils components (like BB1PL and BB1MI in Fig. 5) are used to link the two faces of each channel from the geometrical design with the attached electrical circuit. Their characteristics (conductor material, number of turns, etc.) were set in accordance with the real winding arrangements. For each channel of the SRM two such components are used: the "come" and "go" sides (faces) of the winding.

As it was stated previously at each time two channels (4 coils) are fed by the two corresponding H-bridges. The H-bridges are connected in parallel to the main bus bars, and they are commanded separately, but synchronously. The block diagram of the coupled simulation program is given in Fig. 6. The imposed simulation task is solved by means of time stepping method.



Figure 6: The block diagram of the coupled simulation program

The FEM model of the SRM is embedded in the main SIMULINK[®] program. The analytical model of the drive system is computing at each time step the power switches command signal (PSCS), which are practically setting the values of the resistors from the machine's circuit model. The computations are performed using several constant parameters (CP) as being inputs in the system, respectively the current (*I*) and the angular position (θ) error signal. At every time step data are exchanged between Simulink[®] and Flux 2D. The FEM model is returning to the main program four signals: the phase currents, the electromagnetic torque (*T*), the mechanical speed (Ω) and the angular position of the SRM at that time step.

The main window of the simulation program is given in Fig 7.



Figure 7: The main window of the simulation program

As it can be seen 6 sub-systems (blocks) are controlling the phase currents upon the PWM technique. The commutations of the power switches are set upon the rotor position. Each block is built up using logical, switch and hysteresis blocks, as shown in Fig. 8.



Figure 8: The phase current controller block

The FLUX 2D model of the SRM is embedded in the main program via an S-type function called *Coupling with Flux2d*. Its mask is shown in Fig 9.

terre - cooping) (mask) (link)
Get INPUT from	n Simulink, Put OUTPUT from FLUX2D
arameters	
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SRM	
Flux2d Input	
[Voltage:V1;R	esistance:RA1_1;Resistance:RA1_2;Resistance:RA2_1;Resistance:R
Flux2d Output	
[Torque;Teta;	Current:BA1PL;Current:BB1PL;Current:BC1PL;Current:BD1PL]
Time Step	
0.01	
Initials Conditio	ns
[TETA0=0]	
Memory (Mo)	
300	
300	

Figure 9: The mask of the coupling block

All the control signals computed in SIMULINK[®] and entering this block are multiplexed. The outputs of the field computations are returned to the main program through another multiplexed signal line.

RESULTS OF SIMULATIONS

The main data of the SRM in study are:

- i.) Voltage: 250 V
- ii.) Reference phase current: 40 A
- iii.) Input phase power: 10 kW
- iv.) Phase resistance: 1.2Ω
- v.) Number of turns per phase: 100

Constant velocity was imposed (600 r/min) during the time stepping simulation. The fault tolerance capacity of the SRM was studied in steady-state regime was considered.

The proposed SRM was simulated under different conditions in order to check its fault tolerance capability:

- i.) normal operating mode (reference case),
- ii.) open circuit of one channel,
- iii.) open circuit of one phase,
- iv.) open circuit of two channels from different phases,
- v.) open circuit of one phase and one channel from a different phase (worst case in study).

In all the cases the simulation time 8 ms in no-load conditions. The mean torque developed in normal operating mode was the reference value in this study.

The current and torque waveforms versus time for the healthy and for all the four faulty conditions of the proposed SRM are given in Fig. 10.

As it can be seen in the figure a short transient period is required still the current reaches its maximum value.

In the plots the effects of faults can be observed as missing currents and decreasing torques, due to the faulty windings.

The current and torque plots for the healthy machine operating under normal conditions are given in Fig. 10a. As the machine has higher number of phases and stator poles than the usual 12/8 topology the torque ripples are relatively lower (Ruba 2008c).

If one channel is open (Fig. 10b) due to the missing channel's currents the torque is lower than in the previous case and torque ripple is higher.

When an entire phase is faulty (Fig. 10c) there are moments when the torque is falling to zero, because the load inertia and the resistive torque are nil, at no-load conditions.

In the situation of the faults on two different channels from two different phases, Fig. 10d, the torque ripple is greater.

The worst case in study is the fault of an entire phase, and a second fault on one channel from different phase (Fig. 10e). The torque ripples in this case are the highest.



Figure 10: Current and torque plots of the SRM in study under different faulty conditions

Results concerning the torque development capability of the SRM in study are given in Table 1.

Studied cases	Mean torques [N·m] and percentage of the rated torque
Healthy case	19.93 (100%)
Faulty case 1	19.59 (98.29%)
Faulty case 2	16.16 (81.03%)
Faulty case 3	19.28 (96.71%)
Faulty case 4	13.79 (69.19%)

Table 1: The mean torques of the SRM for all the cases taken in study

The torque ripples are different from a case to another and depend on the fault's severity.

As seen in the Table 1 the proposed fault tolerant 12/14 SRM topology is able to develop torque (around 70% of the rated torque) and continue its movement even at the hardest fault in study, when one phase and one channel from a different phase is damaged. Obviously the torque ripples are the greatest in this case. Of course heating and force distribution issues limit the operation in this faulty case

In the case of the first fault in study, nearly full torque is developed (more then 98% of the rated value). Also high mean torque is generated when two channels from different phases are opened (Fig. 10d).

A solution to improve the torque development of a machine in case of faulted windings is to isolate the defect, and to increase the current in the remaining healthy phases. By this the torque's average value can be held at the same value as in normal operation mode. Unfortunately this solution do not decrease the torque ripples.

Higher currents mean higher temperature and higher losses. Uncontrolled temperature rise can damage the healthy phases, on one side, and on the other, operation at higher currents demand higher power converters.

Hence this solution can be used only if the windings and the cooling system of the machine were designed to support the greater currents and over heating.

CONCLUSIONS

The study demonstrated that increasing the number of rotor poles and stator winding phases, separating the phases/channels, setting new connections between the existing windings, and using a complex control system all provided good solution for the fault tolerant SRM based electrical drive system.

The increased number of rotor poles and the more complex electronic system that drives and controls the machine means of course higher costs. These costs depend on the level of tolerance implemented in the system. Upon the demands of specific applications, the electrical drive system (both the power converter and the machine) can be optimized and a compromise between fault tolerance level and manufacturing costs can be made.

The fault tolerance study of the proposed SRM was carried out upon the results of simulations. The transient regime simulation of the entire electrical drive (the machine and its converter) was performed using the advanced coupled simulation technique (FLUX 2D to Simulink[®]). This way it was taken advantage of the high precision machine analysis capabilities enabled by the FLUX 2D FEM based numeric field computation program and the easy-to-use, but advanced MATLAB/Simulink[®] environment. In Simulink[®] it was very simply to impose different working regimes and faulty cases.

The use of co-simulation techniques offers several advantages:

- i.) It is possible to have full system simulations even with mixed-signal parts.
- ii.) It permits full system simulations reducing verifications and testing costs compared to full laboratory system testing in real hardware.
- iii.) Simulink offers easy-to-use environment for simulations.
- iv.) The use of the most proper simulation program for each system component.

Future works are regarding changes of the machine geometry by new placements and connections of the windings. The different constructions shall be compared by means of co-simulation techniques. The prototype of the best fault tolerant SRM variant is intended to be built up.

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CONCERNING THE SIMULATION OF THE CONNECTION OF THE NO-LOAD TRANSMISSION LINES IN HIGH VOLTAGE NETWORK

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Transmission line, Switching over voltages, Matlab

ABSTRACT

This paper describes a Matlab program designed to compute the switching over voltages which appear when no-load high voltage lines are energized. The mathematical models of the high voltage distribution lines are presented also. The Matlab program is applied for the case of the high voltage distribution lines from the 220kV network of the ST Craiova, for which the characteristic parameters are known.

INTRODUCTION

The values of the switching over voltages appearing when the no-load lines are energized depend on the parameters of the electrical diagram or the equivalent circuit diagram at initial instant. The complexity of the mathematical model depends on the number of characteristics of the switching process and also on the type of electrical diagram used (mono or three phase one). The values of the computed over voltages are very important for the high or very high voltages networks, having the neutral point directly earthed. In this case a mono phase diagram can be used because the processes are analogous to the others phases. Considering the line model with concentrated parameters, the line can be represented by the T or Π quadripole, the resistances being neglected in comparison with the reactance values, as is shown in the Figures 1a and 1b.



Figure 1: Equivalent Diagram: a) T Quadripole; b) Π Quadripole

Corresponding to the steady state operation at 50Hz, the value of the concentrated parameters can be computed by means the impedances having the following expressions:

 \cdot for T quadripol :

$$L_{\lambda} = \frac{Z_{c}}{\omega} tg\left(\frac{\beta l}{2}\right),$$

$$C_{\lambda} = \frac{1}{Z_{c}\omega} \sin\left(\beta l\right);$$
(1)

 \cdot for Π quadripol:

$$L_{\lambda} = \frac{Z_{c}}{\omega} \sin\beta l , \qquad (2)$$
$$C_{\lambda} = \frac{1}{Z_{c}} \omega \sin(\beta l) ,$$

where:

$$Z_c = \sqrt{L_o / C_o}$$

is the line characteristic impedance,

 L_o [H/km] and C_o [F/km] are the line inductivity respectively capacitance per unit length, $\beta = \omega \sqrt{L_o C_o}$ is the phase constant,

 $\lambda = \beta l$ is the electrical length of the line, $\omega = 314 \text{ rad/s}$.

The equivalent inductivity respectively capacitance has the following expressions (Dragan 1975): • for T quadripole:

$$L_e = L_s + L_\lambda ,$$

$$C_e = C_\lambda ;$$
(3)

 \cdot for Π quadripole:

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$$L_{e} = C_{\lambda} \left(\frac{L_{\lambda}}{C_{\lambda}} + \frac{L_{s}}{C_{\lambda}} - \omega^{2} L_{s} L_{\lambda} \right),$$

$$C_{e} = C_{\lambda} \left[1 + \left(1 - \omega^{2} L_{\lambda} C_{\lambda} + \frac{L_{\lambda}}{C_{\lambda}} \right)^{-1} \right],$$
(4)

where L_s is the power supply inductivity. The analytical expressions for the over voltages computations are:

$$u_{c}(t) = \frac{\hat{U}}{C_{e} Z_{e} \omega} \left[\sin\left(\omega t + \psi - \varphi\right) - e^{-\delta t} \cdot S(t) \right], \quad (5)$$

$$S(t) = \frac{\sin(\omega_1 t + \alpha)\sin(\psi - \phi)}{\sin\alpha} + \frac{\omega}{\omega_1}\sin(\omega_1 t)\cos(\psi - \phi)$$
(6)

where ψ is the angle phase of the power supply voltage,

$$\begin{split} Z_e &= \sqrt{R^2 + \left(\omega L_e - 1/\omega C_e\right)^2} ,\\ \delta &= \frac{R}{2L_e} ,\\ \omega_1 &= \sqrt{\omega_0^2 - \delta^2} ,\\ \omega_o &= \frac{1}{\sqrt{L_e C_e}} \\ \phi &= arctg \left(\frac{\omega L_e - \frac{1}{\omega C_e}}{R} \right). \end{split}$$

Considering R=0 and $\psi=0$, the next simplified expression is obtained:

$$u_{c}(t) = \frac{\hat{U}}{C_{e} Z_{e} \omega} (\cos \omega t - \cos \omega_{1} t) ,$$

The amplitude factor of the over voltage at the line end is:

$$k = \frac{\max\left(u_{c}\left(t\right)\right)}{\sqrt{\frac{2}{3}} \cdot U_{n}} = f\left(l, \omega_{1}\right), \ \psi = 0, \qquad (7)$$

The maximum value of the over voltage depends on the angular resonant frequency of the equivalent circuit ω_{oT} or $\omega_{o\Pi}$.

The following expressions for the angular resonant frequency are obtained by successive replacements:

$$\omega_{oT} = \frac{\omega}{\sqrt{1 - \cos \lambda + \left(\frac{X_s}{Z_c}\right) \sin \lambda}},$$

$$\omega_{o\Pi} = \frac{\omega}{\sqrt{\left(\frac{X_s}{Z_c}\right) \sin \lambda + 1 - \cos \lambda}};$$
(8)

From the analysis of the two expressions one can notice that $\omega_{oT} = \omega_{o\Pi}$.

If the line modeling is performed by considering distributed parameters, without transversal compensation, the following analytical expression of the voltage at the end of line can be used:

$$u_{2}(t) = U_{2ss}\left[\cos\left(\omega t + \psi\right) + \sum_{k=1}^{\infty} A_{k} e^{-\alpha_{k} t} \cos\left(\omega_{k} t + \psi_{k}\right)\right],$$
(9)

where

 $u_2(t)$ is the instantaneous value of the voltage at the line end;

 U_{2ss} is the steady state amplitude of the voltage at the end line;

 ψ is the phase angle of the voltage at the end line;

 A_k is the amplitude of the k harmonic per unit of the steady state voltage amplitude;

 α_k is the delay constant of the *k* harmonic of the voltage at the line end;

 ω_{ok} is the angular frequency of the k harmonic.

Among the terms of the infinite string from the above expression, only the first terms has a strong contribution to the maximum value of the voltage. Considering only two first terms (k = 1, k = 2) we will obtain the analytical expression corresponding to the equivalent circuit from the figure $1b - \Pi$ quadripole; for k = 1 the analytical expression corresponding to the equivalent circuit from figure 1a - T quadripole will be obtained. The angular frequency ω_{ok} differs from the $\omega_{oT(\Pi)}$ obtained using the expressions (8). The computed error is smaller as the length of line increases and as the system power decreases.

For the line represented by distributed parameters, the transversal compensation can be done by installing one reactor at the front end of the line. In this case the amplitude of the over voltage depends on the saturation level of the reactor magnetic core. For the circuit breaker equipped with shunt resistor, the over voltage value depends on the resistance value.

THE PROGRAM DESCRIPTION

The Matlab program has been used in order to compute the electrical stresses from the high voltage network of the ST Craiova. The program was designed in an interactive manner which allows the selection of the network and of the faults type (Brojboiu 2005). In Table 1 are presented the computed parameters, applying the designed program, for electrical station North Craiova: a) Işalniţa line:

 $U_n = 220 \text{ kV},$ $S_t = 200 \text{ MVA},$ l = 9.6 km, $R_0 = 0.0674 \ \Omega/\text{km},$ $L_0 = 0.00128$ H/km, $C_0 = 8.8 \cdot 10^{-8}$ F/km; b) Bradu line: $U_n = 400 \text{ kV},$ $S_t = 400 \text{ MVA},$ l = 196.4 km, $R_0 = 0.034 \ \Omega/\text{km},$ $L_0 = 0.00105$ H/km, $C_0 = 1.0884 \cdot 10^{-8}$ F/km; c) Tr. Măgurele line: $U_n = 220 \text{ kV},$ $S_t = 200 \text{ MVA},$ l = 121 km, $R_0 = 0.06875 \ \Omega/\text{km},$ $L_0 = 0.00130 \text{ H/km},$ $C_0 = 8.833 \cdot 10^{-9}$ F/km.

 Table 1 The Computed Parameters

Line	<i>l</i> [km]	ψ	$\max\left(u_{c}\left(t\right)\right)$ [kV]	k	t _{max} [ms]
Icolnito	0.6	$\pi/2$	153.07	1.0956	15
ışannı	9.0	0	275.68	1.97	0.9
Tr.	121	$\pi/2$	150.4	1.076	14.2
Măgurele	121	0	267.94	1.918	1.3
Dradu	106	$\pi/2$	312.77	1.23	16
Diadu	190	0	459.9	1.81	2.4

The Matlab program has been applied to observe the influence of the line length on the over voltages values. The maximum value of the over voltage, the time when the maximum value is reached as well as the amplitude factor k have been also computed. The line was represented as the T or Π quadripole. By analyzing the computed data, was observed the decreasing of the resonant angular frequency as the length line increases as is shown in the Figure 2.

The resonant angular frequency has an influence on the amplitude factor as seen from (7). Regarding the variation in time of the over voltage one noticed, as in (Dragan 1975) that: a) for the ratio $\omega_{oT(\Pi)} / \omega = 1...1.6$ the amplitude factor is given by the third maximum; in the Figure 3 is plotted the graphic $u_{cT} = f(t)$ for

 $\omega_{oT(\Pi)} / \omega = 1.5$, $l = 228 \ km$, $\psi = 0$; b) for the ratio $\omega_{oT(\Pi)} / \omega = 1.6...3$ the amplitude factor is given by the second maximum; in the Figure 4 is plotted the graphic $u_{cT} = f(t)$ for $\omega_{oT(\Pi)} / \omega = 1.8$, $l = 178 \ km$, $\psi = 0$; c) for the ratio $\omega_{oT(\Pi)} / \omega > 3$ the amplitude factor is given by the first maximum; in the Figure 5 is plotted the graphic $u_{cT} = f(t)$ for $\omega_{oT(\Pi)} / \omega = 3.5$, $l = 68 \ km$, $\psi = 0$.



Figure 2: The Angular Frequency vs length





Figure 4: The $u_{cT} = f(t)$, $\omega_{oT(\Pi)} / \omega = 1.8$



Figure 5: The $u_{cT} = f(t)$, $\omega_{oT(\Pi)} / \omega = 3.5$

The variation of the amplitude factor depending on the line length is plotted in Figure 6.



Figure 6: The variation k = f(l): solid line – T quadripole, dotted line - Π quadripole

From Figure 6 can be noticed that large differences between the values result for high values of the length line; the values for the T quadripole are bigger than for the Π quadripole.

Regarding the influence of the phase angle, the program allows to automatically change this value. As expected, the maximum values of the over voltage is reached for the phase angle values near the zero value.

In the Figures 7 and 8 are plotted the variation of the $u_{cT} = f(t)$ for two values of the length line.



Figure 7: The variation $u_{cT} = f(t)$, l = 10 km



Figure 8: The variation $u_{cT} = f(t)$, l = 100 km

Regarding the exact computation of the over voltage amplitude, the references in the field recommend replacement of the lines with l = 200...300 km , by the T quadripole, while the lines with l > 300 km by the Π quadripole.

The computed data using this Matlab program has been used to assess the electrical stresses in the high voltage network and to choose the appropriate circuit breaker corresponding to the fault regime also.

CONCLUSIONS

The Matlab computation program presented in this paper allows the evaluation of the maximum values of the switching over voltages appearing at the no-load high voltage lines. The influence of the length line and the phase angle values on the over voltage amplitude has been also studied. The program has been applied for the case of the high voltage lines from ST Craiova for which the rated parameters are known.

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DESIGN AND IMPLEMENTATION OF AN INTERACTIVE INTERFACE FOR POWER PLANT SIMULATION

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KEYWORDS

Computer Aided Design, Graphical Model Builder, Brayton and Rankine Cycle, Powerplant Simulation

ABSTRACT

A large number of useful software was written at a time when graphical user interfaces were not the norm. By current standards these programs are often dismissed as being difficult to use and are ignored. Brakine is one such program. Brakine is a powerful design and simulation system of arbitrary energy systems that operate on the thermodynamic principles of the Brayton and Rankine cycles. It suffers from a very tedious user interface and has fallen largely out of use. This project creates a new visual user interface for Brakine that facilitates the design of the simulation by providing functionality to draw the entire simulation on screen. The tedious task of generating the text input file and reading the text output file is taken away from the user. The graphical user interface generates the correct input file for the simulation by taking into account the inter-connectivity of the components that have been drawn on the screen and the simulation parameters that have been assigned to these components. The results of the simulation are displayed by labelling the connections between components. This aids in the overall understanding and interpretation of the simulation.

1. INTRODUCTION

One of the greatest contributing factors for the failure of software in the marketplace, is a badly designed userinterface (Hobart, 2001). If end-users feel that the learning curve of the software is too steep they will quickly abandon the product in search of something that is more user-friendly. Many valuable programs are never utilized to their full potential because of steep learning curves. The reason why such a large number of programs end up unusable is because their user-interfaces were implemented as an after-thought, instead of being integrated tightly into the development cycle.

With the introduction of Windows as a world-wide operating system, end-users have come to expect a userinterface that is visually driven. Programs that operate in text-mode are judged to be archaic and are quickly dismissed. Unfortunately, there are many useful and relevant programs that were programmed when a text-mode user-interface was still the norm. A new visually driven interface must be designed for these types of programs before they fall completely out of use.

The aim of our work is to design and implement an interactive visual user-interface for *Brakine* (Roy-Aikins, 1995). Brakine is a versatile design and simulation system of arbitrary energy systems that operate on the thermodynamic principles of the Brayton and Rankine cycles (Cengel and Boles, 2006). It is text-mode driven and suffers from a very tedious user-interface. As such its use is severely limited and it has never been introduced into the classroom. The new visual user-interface will resolve some of the biggest obstacles a user experiences when working with the Brakine simulation and will facilitate the drawing of engineering diagrams so that the entire simulation, including the results, can be displayed on screen in an interactive manner.

The rest of this paper is organized as follows. We start by presenting an overview of the Brakine software and its limitations. Section 3 presents related work and in section 4 we delve into the architecture of our solution. In section 5 we provide a description of JGraph. Section 6 looks at some key functionalities of our software and 7 examines the results and limitations. Finally section 8 concludes our work and provides suggestions for future work.

2. Background

The Brakine simulation program was written in Fortran and designed at a time when graphical user interfaces were not the norm. As such it is text-mode driven and relies on the user to type an input file that specifies information for the simulation. The results of the simulation are then written to an output file.

It is the generation of the input file that poses the biggest problem. Generating the input file is a daunting task because the input file has to adhere to a very strict structure and the amount of information that the user has to specify can also be overwhelming. The entire design of the system including the inter-connectivity between components, all simulation parameters and other information such as scheduled data have to be typed out. This

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is a very tedious and time consuming process. It is also a very error-prone process.

Before the input file can be created the user draws a mechanical engineering diagram of the system that will be simulated. This has to be done on paper because there is no functionality in the simulation program to allow the user to draw diagrams. If the drawing is accidentally lost or misplaced it becomes very difficult to visualize the design of the system, because the input file by itself is rather obscure.

The simulation software was originally designed as a teaching tool for mechanical engineering students because commercial software was too expensive. However, students could simply not overcome the very steep learning curve of this tool. For these reasons the software has fallen largely out of use.

In this paper we present the design and the implementation of an interactive interface that will allow the user to draw the mechanical engineering diagram on the computer. The input file for the simulation program will be generated automatically based on the diagram that the user has drawn and the properties the user has assigned to the mechanical engineering components via the graphical user interface. This will remove the burden of typing the input file from the user. Furthermore the interactive interface will display the results of the simulation by labelling the connections between components so that the user can visualize the outcome of the simulation. By placing great emphasis on making the interface userfriendly the Brakine simulation software can be brought back into use.

3. Related Work

Several computer aided design tools for power plant simulation have already been reported in the literature. One of these initiatives is called Modular Modeling Systems Model Builder (MMSMB) (McKim and Matthews, 1996). With this program a user can quickly build a simulation by selecting from a library of pre-configured power plant components to dynamically simulate their operation. Simulation code is automatically generated by taking the connectivity and parameters of different components into account. Another power plant simulation tool that was developed recently is called Power-Sim (Kim et al., 2005). It is targeted at the Korean market and aims to be a more flexible power plant design tool than MMSMB by allowing the user to integrate new custom-made components into the power plant component library. The modeling tool Modelica has also been used as a platform for power plant simulation, however the work of (Casella and Leva, 2003) is incomplete as many components such as compressor, turbine or combustion chambers still need to be developed. The fundamental difference between our work and related work is that their scientific visualization of the simulation was planned and integrated into the design of the program from the start of the development cycle. In our case, we

are integrating a visualization tool with a simulation program that was not designed for one, and report on the issues that arise in such an endeavor. One of the first problems is identifying the best tools that will facilitate the integration of the visualisation functionality.

Generating the correct input file for the simulation based on the diagram the user has drawn and the properties the user has assigned requires knowledge of the structure that the input file must adhere to and is unique to this project. However, a lot of previous work has been done in generating an interactive user-interface that facilitates the drawing of diagrams.

There are numerous *Java* libraries that assist in the drawing of diagrams, each with their own advantages and disadvantages. The leading commercial libraries are *yFiles* (yWorks, 2009) and *Tom Sawyer Software* (Tom Sawyer Software, 2009). They provide numerous layout algorithms as well as a plethora of other features. They are however expensive and the source code is not available meaning that they cannot be customized.

In terms of open-source software libraries there are also a lot to choose from. The Java Universal Network/Graph Framework (O'Madahain et al., 2003) is an open-source software library designed to support the modelling, analysis, and visualization of data that can be represented as graphs. Its emphasis is on mathematical and algorithmic graph applications pertaining to the fields of social network analysis, information visualization, knowledge discovery and data mining. It is ideal for fast rendering of very large graphs but it is not suitable for this project because even though the mechanical engineering diagram that the user draws is essentially a graph, a lot more detail and control is needed for the design and layout of the diagram than the library provides.

Another very recent Java library that is rapidly gaining popularity is *Prefuse* (Pendleton et al., 2007). Prefuse is a Java-based toolkit for building interactive information visualization applications. It provides optimized data structures for tables, graphs, and trees, a host of layout and visual encoding techniques, and support for animation, dynamic queries, integrated search, and database connectivity. Once again, it is targeted at very large graphs and some of the features like optimized data structures are not required for this project. Hence is also not suitable.

There are many other Java graph drawing libraries that are available but they either have very poor documentation or are no longer being developed.

A notable exception to this is *JGraph* (Alder and Benson, 2001). JGraph is a flexible *Swing* graph visualization and layout library. JGraph is specifically orientated towards design layout, like the popular *Microsoft Visio* (Microsoft, 2007). It is probably the most well known open-source graph visualization library currently available and has a very vibrant user community. It is actively maintained and comes with an excellent free user manual and numerous example programs. The community forum is also very active and posts are made on a daily basis.

JGraph has been used for numerous applications that

are related to this project in terms of interface design.

Aigner and Mikisch (Aigner and Miksch, 2004) made use of the JGrpah library to develop an interactive visualization method for computer supported protocol-based care in medicine.

JGraph was also used by (Hanish et al., 2004) to create a tool for interactively exploring the meaning of expression experiments in context of biological networks.

Valyi (Valyi and Ortega, 2004) used JGraph to create an open source simulation platform dedicated to systems ecology and emergy studies called *Emergy*. Emergy is an efficient graph sketcher that allows users to draw an energy diagram while providing an intuitive drag and drop interface, high standard graphical features and an extensible interactive and multilingual help system.

Reyes (Reyes, 2004) created a prototype *StreamIT Graph Editor* using the JGraph library. *StreamIT* is a language for the development of streaming applications that has a hierarchial and structural nature that lends itself to a graphical programming tool. The StreamIT Graph Editor provides intuitive visualisation tools that allows developers to work more efficiently by automating certain processes.

Commercial companies have also used JGraph in their applications.

Clearly the JGraph library is well suited to design a very user-friendly and flexible interactive interface. For this reason it was the library of choice for this project.

To our knowledge there is currently no open-source project that can be used to simulate arbitrary energy systems based on the Rankine and Brayton cycle, like the Brakine program can. For this reason no attempt has been made to design a graphical user interface for such an application as an open-source community project. There are however commercial applications that perform a very similar function to what this project aims to achieve. The company that has been at the forefront of designing thermal engineering software for the power and cogeneration industries since 1987 is Thermoflow Inc (Thermoflow, 2009). Thermoflow's first product, GT PRO, has grown to become the world's most popular program for designing gas turbine-based plants. However it is another one of their products, Thermoflex, that is of particular interest to this project. Thermoflex is a modular program with a graphical interface that allows for the assembly of a model from icons representing over one hundred different components. The program covers both design and off-design simulation, and models all types of power plants, including combined cycles, conventional steam cycles, and repowering. It can also model general thermal power systems and networks.

Initially Brakine was written as an alternative to the products that *Thermoflow* provides. The ultimate goal was to provide similar flexibility in design that Thermoflex currently offers. The interactive interface that Thermoflow provides in many ways is a benchmark for this project (see Fig 1).



Figure 1: Screenshot of Thermoflex Software

4. ARCHITECTURE OVERVIEW

To understand how the graphical user interface that we created interacts with the Fortran simulation program, it is best to look at the flow of data between these two programs (see Fig 2).

The graphical user interface generates an input file for the Fortran simulation based on the components that have been dragged into the document, the connectivity between the components and the simulation data that the user has assigned to the components. Once the input file has been generated the user runs the Fortran simulation program using the generated input file as the input file for the simulation. The Fortran simulation program produces an output file containing the results of the simulation. This output file is parsed via the graphical userinterface and the results of the simulation are displayed by labelling the edges between the different components on the screen.



Figure 2: Flow of Data

In this way the difficult and tedious task of creating the input file is taken away from the user. Furthermore, by labelling the edges between components with the correct simulation results the user can better understand the outcome of the simulation.

The Brakine simulation software expects the input file to follow a very strict order and structure. The breakdown of the structure can be found in (Roy-Aikins, 1988). A snippet of data for a text input file for a jet engine simulation is given in Table 1. This kind of input file is now automatically generated by our graphical user



Figure 4: Model View Controller

interface. Most of the information that is required by the input file is extracted from the components on the screen, by considering how a user connects components together, and by capturing simulation data via input dialogues.

To display the results on screen and to label the connections between components with the relevant results the output file of the simulation program is parsed. What is of particular interest to the user is the mass flow ratio, the total pressure and the total temperature between two components. Regular expressions (Friedl, 2006) are used to extract this information from the output file. A snippet of an output file that is generated by the original Fortran program is presented in Table 2. The visual interpretation of these results generated by our program is presented in Fig 3.

5. JGRAPH ARCHITECTURE

JGraph complies with all *Swing* standards, both visually and in its design architecture (Benson, 2001). As such, it is built around the Model-View-Controller (MVC) design pattern (see Fig 4).

The Model-View-Controller pattern is used when the user interface needs to be separated from the functional core of the program (Buschmann et al., 2001). By separating the user interface from the core functionality, several different views of the model can be displayed. For example, in JGraph the logical graph that is specified in the model can be displayed in various different ways at different levels of detail simultaneously.

The Model-View-Controller architecture divides a problem into three areas: processing, output and input. This means that the model contains the core functionality and data, the view displays information to the user and the controller handles user input. The important concept in the MVC pattern is that the model is totally independent of specific output representations or input information(Buschmann et al., 2001). The view obtains the data that it wishes to display from the model and multiple views of the model can exist at any point in time. The controller receives input events, usually mouse or keyboard, that are then translated into service requests for the model and view. In this way the view and controller work together to make up the user interface. Table 1: Code Snippet of a Sample Input File to Simulate a Jet Engine PROGRAM TITLE//// DP SI KE FP -1 -1 -1 2 1 7 2 3 7 .6 42.5 .7 42.5 .8 42.5 .85 28.5 .9 14.5 .95 .5 .97 -5. 1. 3 1 7 2 3 5 .6 .13 .7 .115 .8 .1 .8 .05 .8 .05 .9 .05 1. .05 1. -1 INTAKE S1,2 D1-5,78,278-279,344 COMPRE S2,3 D6-17 R51 V1,2,6 A86-106 PREMAS S3,10,3 D18-23,268 A107-127 PREMAS S10,11,12 D80-85,269 A128-148 BURNER S3,4 D24-27 R69 MIXEES S4,11,5 D317 TURBIN S5,7 D43-57,341,343 V2,2,44 W3,2,43 DUCTER S7,8 D58-62,149 NOZCON S8,9,1 D63,79 CODEND T64-GE-415 DATA//// !GAS TURBINE CYCLE ! INTAKE 1 0 2 0 3 0 4,99 5 -1 78 -1 !COMPRE 6.85 7 1 8 12.5 9.82 10 -1 11 1 13 -1 8 12.5 14.9 15 -1 16 1 17 -1 ...



Figure 3: Labelling of Edges with Simulation Results



Figure 5: (a) Simple Diagram (b) Graph Topology of the Simple Diagram

The JGraph model provides the data for the graph. It consists of connection information and cells which may be vertices, edges or ports. The connection information that is stored in the model is defined using ports because they make up an edge's source or target (Alder, 2001).

The graph structure provides methods to retrieve the source and target port of an edge and to return the edges that are connected to a port. Refer to Fig 5 for an example of a graph topology for a basic diagram.

Following the JGraph architecture every mechanical engineering component as well as all connections between components can be called cells, because a cell is the superclass of a vertex, edge and port. Cells have attributes that define visual information such as the size,



Figure 6: Relationship Between Cells and Vertices, Edges and Ports.

position, shape and rotation of the cell. The attributes of a cell are stored in an attribute map. The maps provide an easy and convenient way to customise the display and behaviour of any cell, and hence any vertex edge and port (because a cell is the superclass). For the purpose of this project a cell, if it is a vertex, also stores an icon representing a particular mechanical engineering component.

To store data that is not needed for rendering, a cell may also hold a reference to userObject. A userObject is of type Object and in this way provides a way to associate any object with a cell. The link between a cell and simulation data for that cell is established via the userObject.

In summary, a cell may either be a vertex, a port or an edge and a cell contains an attribute map that defines how it is to be rendered. For the purpose of this project, a vertex represents a mechanical engineering component and an edge represents a type of connection between two mechanical engineering components (see Fig 6).

```
Table 2: Code Snippet of a Sample Output File for
a Jet Engine Simulation
... ***** TURBINE 1 PARAMETERS *****
CNSF = .10000E+01 ETASF = .96437E+00
TFSF = .10000E+01
DHSF = .13827E - 03
TF = 48.856 ETA = .85000 CN = 1.000
AUXWK = .35000E+07 DELHN = .11500E-05
ARATIO = .1300E+01
DELHT = .62000E-01
**** CONVERGENT NOZZLE 1 PARAMETERS
****
Area = .5310 Exit Velocity = 67.66
Gross Thrust = 1016.54
Nozzle Coeff. = .97021E+00
Scale Factor on above Mass Flows,
Areas, Thrusts & Powers = 1.0000
Station F.A.R. Mass Flow Pstatic
Ptotal Tstatic Ttotal Vel Area
1 .00000 15.194 1.00000 1.00000
288.00 288.00 .0 *****
2 .00000 15.194 ***** .99000 *****
288.00 ***** *****
3 .00000 14.434 ***** 12.37500
***** 650.47 ***** *****
4 .02019 14.726 ***** 11.50875
***** 1350.00 ***** *****
5 .01918 15.485 ***** 11.50875
***** 1318.40 ***** *****
6 .00000 .000 ***** .00000 *****
.00 ***** *****
7 .01918 15.485 ***** 1.01846 *****
821.04 ***** *****
8 .01918 15.485 ***** 1.00863 *****
821.04 ***** *****
9 .01918 15.485 1.00000 1.00863
819.03 821.04 67.7 .5310
10 .00000 .760 ***** 12.12750 *****
650.47 ***** *****
11 .00000 .760 ***** 12.00623 *****
650.47 ***** *****
12 .00000 .000 ***** .00000 *****
.00 ***** *****
```

```
• • •
```

6. SOME KEY FUNCTIONALITIES

Long-term persistence is the technical term given to the concept of saving the state of a program and reloading it at a later stage. Traditionally, Java serialization was used to achieve long-term persistence. Serialization works by writing the entire state of an object into a byte stream. This means that to save a program, all the important objects that make up the state of the program are written to a byte stream. The byte stream can later be deserialized in such a way that the state the program was in when it was saved is recreated (Winchester and Milne, 2009).

There are several problems with this approach. The mechanism used to deserialize an object stream relies on the internal shape of the classes that make up the objects to remain unchanged between encoding and decoding (Winchester and Milne, 2009). This means that any changes to the classes, such as adding or renaming some fields or methods between the time that the program was saved and retrieved, will cause deserialization to fail. Clearly serialization is not a viable solution for this project because a tool such as a graphical user interface is likely to undergo many refinements and extensions in the future.

To circumvent this problem an XMLEncoder was used. An XMLEncoder takes a very different approach to long-term persistence. Instead of storing a bit-wise representation of the field values that make up an object's state, the XMLEncoder stores the steps necessary to create the object through its public API (Winchester and Milne, 2009). The advantage is that many changes can be made to the implementation of a class while preserving backward compatibility through the API. For a thorough discussion on XMLEncoding refer to (Milne, 2009).

Drag and drop refers to functionality that allows a user to click on a mechanical engineering icon and drag and drop it anywhere into the document. While dragging a preview of the icon appears at the location of the cursor. This is commonly also known as drag and ghost since the preview icon is usually somewhat transparent. The drag and ghost functionality was implemented to make the graphical user interface more user-friendly.

To store simulation data the concepts described in the *JGoodies*(Lentzsch, 2009) project, such as data binding and data validation were used. The fundamental concept behind JGoodies Binding is that it synchronizes object properties with Swing components. It also helps to represent the state and behavior of a presentation independently of the GUI components used in the interface. JGoodies Validation on the other hand helps to validate user input in Swing applications and to report validation errors and warnings.

In this project each mechanical engineering component is represented by an object that exposes all simulation properties associated with that component through getter and setter methods. The data for a component is captured by a dialog box. However, before the data is accepted it is passed to a special validator object. Each



Figure 7: How Simulation Data is Stored.

mechanical engineering component has its own validator. The validator uses regular expressions to validate that the user input conforms to the expected input. If the data does not conform the user receives immediate feedback through the dialog box, because the input fields that contain errors turn red (see Figure 7).

7. RESULTS AND LIMITATIONS

Arbitrary energy systems can be visually drawn with a high degree of precision and flexibility. Flexibility and generalisation is achieved in part by using the most elementary mechanical engineering components as building blocks for the system. More complex components are created by combining the elementary building blocks.

The graphical interface is modelled on popular graph drawing programs such as Microsoft Visio. Conventions used in established software packages are followed to make the software more user friendly. With this in mind, the engineering components are represented by icons in the toolbar, which can be dragged and dropped anywhere in the document window. Components are selected by clicking on them, or by dragging a marquee selection window. Multiple components can be selected/deselected by following the Microsoft Windows XP convention of holding down the Ctrl button and clicking. Zoom functionality allows the user to zoom out to get a birds-eye view of the design or to zoom in on particular regions. Connections between components can start and terminate at any location on the component. This is significant because there is meaning associated with where a line terminates on a component. All engineering line styles are supported to represent the connections between components. The line styles differ in color, dash pattern and thickness. Air connections and fuel connections are represented by parallel lines. The line styles differ in thickness to ensure that they will be distinguishable from one another even if printed in black and white. A grid can also be displayed to make the alignment of components easier.

Several design patterns have been used to maintain a clean separation between the view (the graphics the user interacts with) and the model (the relationship between components and their properties). The design patterns further facilitate easier maintenance and extension of the system.

The entire state of the program, including the graphics,

component properties and simulation results can be saved to file and recalled at a later stage.

The properties of components that previously had to be typed into a file are now captured by dialog boxes. The dialog boxes contain input hints that explain what the input fields mean and in what format the input is expected. The dialog boxes are directly associated with the graphical mechanical engineering components, which allows the user to visualize the impact the properties of a particular component should have on a system, by considering the connections between components.

The custom router written for this project, to draw parallel lines between the source and target components orthogonally, has been accepted by the JGraph community as a valuable contribution and is available on the JGraph Community Forum.

8. CONCLUSION AND FUTURE WORK

We managed to transform the Brakine software into a useful and versatile simulation program by creating a new intuitive graphical user interface that links seamlessly with the original Fortran program. However, there is still a lot of work that can be done to further improve the usability of the software. The bulk of the future work should focus on the following:

• JUnit Tests

A comprehensive test suite has to be written for the entire project. This will not only find bugs in the current implementation but will ensure that any future modifications do not break the existing code base.

• Support for Printing

Printing support still has to be coded. This will involve implementing the Java Printable and Pageable interfaces. Care has to be taken to ensure that diagrams scale and fit onto a page.

• Automatic Generation of Brick Data Indices Currently the user is still required to keep track of a lot input information for the simulation that could be generated automatically. This is particularly the case with brick data indices. More information on what brick indices are and what role they play in the Brakine simulation program can be found in (Roy-Aikins, 1988).

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THE INFLUENCE OF THE SAMPLING PERIOD ON THE PERFORMANCE OF THE REGULATION BY DTC OF THE INDUCTION MOTOR

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KEYWORDS

Induction motor, DTC, sampling period.

ABSTRACT

The regulation by DTC of the induction motor is a quite "natural" method, being much lighter, as mathematical support, than the vector control, regardless the type of field considered for orientation. Despite its simplicity, the practical implementation of the method rise serious problems, mainly due to the fact that the sampling period for regulation pourposes is right the minimum PWM period of the inverter which supplies the motor. This why, without involving powerful command systems, the results can be far for the expectances. The paper deals with the simulation of such regulation system and highlights the importance on the performances of the sampling period.

INTRODUCTION

The direct torque control (DTC) of the induction motor represents an alternative to the well known vector control. This control strategy was developed due to the necessity, for certain applications, of avoiding the precise position or speed transducer, or currents loops, required by the vector control schemes. Basically, the DTC of the induction motor controls the speed and the amplitude of the estimated stator flux, by the mean of the stator voltage applied to the motor by a voltage source inverter. The two magnitudes (amplitude and speed of the stator flux) are controlled in order to maintain constant the flux amplitude and to obtain the desired electromagnetic torque.

It is necessary to have an estimation of the stator flux and this could be obtained based on the applied stator voltage and measured stator currents:

$$\underline{\Psi}_{s} = \int \left(\underline{u}_{s} - R_{s} \cdot \underline{i}_{s} \right) dt \tag{1}$$

where \underline{u}_s and \underline{i}_s are the space vectors of the stator voltage and stator current respectively:

$$\underline{u}_{s} = u_{s\alpha} + ju_{s\beta},$$

$$\underline{i}_{s} = i_{s\alpha} + ji_{s\beta},$$
(2)

both referred to the stationary reference frame $\alpha - \beta$ fixed to the stator.

Also, the electromagnetic torque developed by the induction motor must to be estimated. This can be obtained based on the α - β components of the stator flux resulted from (1) and the measured stator currents components from (2):

$$T_e = \frac{3}{2} p \left(\Psi_{s\alpha} \cdot i_{s\beta} - \Psi_{s\beta} \cdot i_{s\alpha} \right)$$
(3)

where *p* is the number of pairs of poles of the machine.

As the inverter states are discrete and consequently the supplied voltages are not sinusoidal waves, the circle of the ideal locus of the stator flux space vector must be reconstituted as precise is possible, in order to avoid high currents and torque ripples. However, this could be done by using the only six non-zero space vectors and the two "zero" space vectors available as output of the inverter (Vas 1998), as are depicted in Figure 1. Figure 2 depicts as example the topology of the inverter that determines the position \underline{u}_2 of the stator voltage space vector.



Figure 1 The Stator Voltage Space Vectors

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Figure 2 The Inverter's Topology for Obtaining the Voltage Space Vector \underline{u}_2

Depending on the sector (Figure 3) where the stator flux space vector is and on the requested action, the next topology of the inverter is chosen in accordance with the commutation table (Table 1).



Figure 3 The Six Sectors of the Plane $(\Psi_{s\alpha}, \Psi_{s\beta})$

The requested action refers to the neccessary evolution of the stator flux as amplitude and speed.

Table 1 The Commutation Table for DTC Control

$ \Psi_s $	Te	Sector					
		1	2	3	4	5	6
\leftarrow	\leftarrow	<u><i>u</i></u> ₂	<u>U</u> 3	<u>u</u> 4	<u>u</u> 5	<u>u</u> ₆	\underline{u}_1
\rightarrow	0	<u>u</u> 7	<u>u</u> 8	\underline{u}_4	<u>u</u> 8	<u>u</u> 7	\underline{u}_8
\rightarrow	\downarrow	<u>u</u> ₆	<u><i>u</i></u> ₁	<u>u</u> 2	<u><i>U</i></u> ₃	<u>u</u> ₄	<u>u</u> 5
\leftarrow	\leftarrow	<u><i>u</i></u> ₃	<u>u</u> ₄	<u>u</u> 5	<u>u</u> ₆	\underline{u}_1	\underline{u}_2
\rightarrow	0	<u>u</u> 8	<u>u</u> 7	<u>u</u> 8	<u>u</u> 7	<u>u</u> 8	<u>u</u> 7
\leftrightarrow	\downarrow	<u>u</u> 5	<u>u</u> ₆	\underline{u}_1	\underline{u}_2	<u><i>u</i></u> ₃	\underline{u}_4

The choice of one of the null vectors \underline{u}_7 or \underline{u}_8 is done having in mind the reduction of simultaneous commutations and consequently, the switching looses in the inverters legs.

As the necessary supplying voltage and therefore the inverter's topology is determined at each sampling period, it is obviously that this one is desired to be as small as possible. If for simulation it is possible "everything", for the real time control, the limitations of the control system must be considered, even it is a DSP based one.

THE SIMULATION OF THE SYSTEM

By using the Simulink libraries previously developed (Ivanov 1998), the model of the driving system, Figure 4, was relatively simply developed.

The most accurate results could be obtained, as can be easily previewed, by choosing a small simulation step. The Figure 5 depicts the results of the simulation with a fixed simulation step of 100μ s. The locus of the flux space vector (a) and the phase currents (b) were detailed for about one period during a step start, in order to highlight the successive commutations determined by the Commutations Table.

The results are quite acceptable due to the fact that the two hysterezis controllers (flux and torque) switch with periods larger than the sampling one, as can be seen in Figure 6. Consequently, the phase voltage plotted in Figure 7 is rich in pulses and the current waveform (Figure 4b) is acceptable.

However, this step is too small for the possibilities of the control board DS1102 that will be used to experimentally test the control. This why, the simulation step size was increased to 500 μ s, as has been estimated that could be a feasible value for the real time control. The results of these simulations are depicted in Figure 8, for a similar regime as in Figure 5. It could be easily noticed the quite disturbed shape of the phase current, due to the reduction to about 2 kHz of the switching frequency of the inverter, as can be seen from the Figure 9, where the phase voltage is plotted.



Figure 4 The Simulink Model of the Driving System with Induction Motor and DTC





Figure 5 Simulation Results for fixed 100 µs Simulation Step of: a – the Locus of the Stator Flux Space Vector; b – Phase Currents



Figure 6 Outputs of the Flux Controller (a) and Torque Controller (b)



Figure 7 The Phase Voltage for Fixed 100 µs Simulation Step



Figure 8 Simulation Results for Fixed 500 µs Simulation Step of: a – the Locus of the Stator Flux Space Vector; b – Phase Current



Figure 9 The Phase Voltage for Fixed 500 µs Simulation Step

EXPERIMENTAL RESULTS

The hard of the testing stand is a DSP based control allin-one board dSPACE GmbH, DS1102. Mainly, the DSP board is equipped with a six channels PWM generator, an interface dedicated to incremental encoders, four A/D channels and four D/A channels. As can be foreseen, these main hardware facilities are quite enough for the development of a simple testing stand. Additionally, thanks to the advantages of the friendly interface supplied by dSPACE GmbH between his DS1102 DSP board and the Matlab-Simulink[®] environment, it is possible the quick implementation of the control algorithms and the interfacing of the sensors.

Using this friendly interface supplied by dSPACE, making only slight changes in the simulation diagrams, the experimentation of different control schemes requires less effort than any other experimentation platform (Ivanov 1997; Ivanov 2003). Basically, the structure of the Simulink control diagram rests as in simulations, only the blocks specific to the interfacing with the power system having to be added. These blocks substitute the models of the inverter and of the motor, as can be seen in Figure 10.





The experimental results were, as could be easily anticipated, not very satisfactory, an example being depicted in Figure 11, where a period of the phase current is plotted.



Figure 11 Phase Current with 500 µs Sampling Time

In order to increase the switching frequency of the inverter without decreasing the sampling period, on one hand, the switching table and on the other hand, the bipositional flux controller and tri-positional torque controller, were replaced by continuous controllers, as can be seen in Figure 12.



Figure 12 The Simulink Model of the Driving System with Induction Motor and DTC without Commutation Table

This allow the generation of the instantaneous values of the preset phase voltages, thus being possible to use a higher switching frequency, even with a sampling period of 500 μ s, due to the advantage of the DS1102PWM unit which uses its own frequency to generate the PWM pulses. As the power part of the inverter consists in MOS transistors, capable to switch at tens of kHz, in simulation it is no more necessary to consider a model for the inverter and the load will act depending on the instantaneous mean value on switching period (about 30 μ s). Experimetal tests will be developed in order to test to proposed control diagram.

CONCLUSIONS

Due to the very basic principles of the classical DTC for induction motor, the switching frequency of the supplying inverter is at most the sampling frequency of the signals necessary for control. Because of this, the performances highly depend on the sampling period which must be as small as possible.

When moderate powerful real time control systems are used, the classic DSP control, based on commutation

table leads to insatisfactory results. The control has to be ameliorated in order to allow greater switching frequency, nondependent by the sampling frequency.

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Configurable FPGA-Based Firing Circuit for Single/Three Phase AC Controller

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Abstract

In this paper, a configurable single chip firing circuit for three phase motor speed control based on Field Programmable Gate Array (FPGA) hardware architecture is presented. The proposed circuit is designed, implemented and tested using MAX II PLD chip (EPM1270F256C5 device). The system has the advantages of being simple, flexible and low development cost with built-in self test. The experimental results carried out using Altera development kit showed that the proposed scheme works properly.

I. Introduction

n the last decades, the production of static power electronics switches has been plentiful and diverse. Some of these switches are GTO's biboplar power transistors, MOSFET's, IGBT's and MCT's [1,2]. Even with these devices, the basic thyristor still constitutes a robust, simple and economical devices, that has many applications. Thyristors are widely used in ac voltage controllers for control of power in both AC and DC systems. This is due to their several advantages such as relatively small size, low losses and fast switching. Apart from many uses, ac controllers are industrial heating, light control, transformer tap changing, ac to dc conversion, reactive power compensation and starting as well as speed control of AC motors [1-4]. The main control technique used in ac controller is the phase angle control technique (PAC). The circuit of PAC consists mainly of two antiparallel thyristor switches, connected in series with each line of the ac supply. PAC is low in cost, simple and by which a large amounts of electric power can be economically controlled. The most main part of the PAC circuit is its firing circuit.

In this paper a new scheme is developed and described, for the thyristor firing circuit. The scheme has the advantages of being simple, flexible and low development cost with built-in self test. Also the scheme can be used for single phase and three phase PAC applications.

II. Scheme Development

As shown in the functional block diagram of Fig.1 the single chip firing circuit scheme is operated by 66 MHz master clock and has a system reset input for system initialization.

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The zerocrossing (squared-up supply frequency) input received from one of the power line phases is used to generate the other two phases. The circuit outputs six different pulses for the positive and negative half-cycles of the three phases. The circuit provides self-test feature as system diagnosis routine. It generates the three zerocrossing digital pulses corresponding to the three phases internally. Moreover, a one Hz pulse ouput is produces and connected to a light emmiting diode (LED) so that its visual blinking is indicating that the circuit is responding and functioning properly, specially during the configutration and programming down loading. The firing angle phase shift is preselected to a default maximum value of 180°, during the initialization phase. This phase shift can be decreased in steps via an external switch to the minimum value of 0° degree. The full block diagram of the proposed firing scheme composed of six different units:

- Timing clocks generator.
- One and 60 Hz circuit.
- Firing angle phase shift circuit.
- Positive / Negative delay circuit.
- The phase generator.
- The main firing circuit unit.

The timing clocks generation unit is responssible for initializing the system, generating several clock pulses used for synchronization purposes, produces the enable signals and loads the proper time constants that are required by the other modules. The one and 60 Hz circuit has two functions for board self-testing purposes. It generates the one second blinking pulse which is connected to the LED indicating that the board is responding to the configuration programming during software down loading. The other one is the artificial 60 Hz zerocrossing that enables the user to test board the circuit board without connecting the firing circuit to the power supply. It is composed of several divide by N cascaded counters and controlled by the timing circuit.

The firing angle phase shift generator unit is to produce the required time delay(α) between the zerocrossing of the particular line phase and the generated firing pulse in degrees. The phase shift ranges from 0° degree to 180° and in approximatly 0.71° resolution steps. The delay steps are controlled by an external push-botton switch (CNT_EN) which in turn, decrements another counter where its contents is used as a time constant for the phase shift counter.

The POS/NEG delay circuit is introduced to generate a certain short time dealy between the rising and falling edges of the positive and negative firing pulses for the

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corresponding phase respectively. This time dely is shown in the timing diagram of Fig.2. This introduced short time delay will prevent the short or open circuits on the power side caused by the high state overlapping due to the opto-couplers time delay response. The delay time depends on the specifications of the opto-couple used. It is in the range of tens of microseconds, therefore, this time delay is kept flexible and can be easily modified by the user to make the firing circuit compatible to any type of opto-coupler switch used.

The phase generation circuit task is to produce internally the other two zerocrossing signals representing the phases Y and Z from the external phase X or from the internal artificial phase in the case of the self test mode . It is mainly composed of several cascaded counters that generate 120° phase shift for both positive and negative half cycles for Y and Z phases. The firing circuit generation unit is considered as the heart of the proposed system. Its main task is to generate the six firing pulses for the positive and negative of the three phases. It is triggered by the external phase applied to the firing chip and controlled by the timing circuit. In the self-test mode, the circuit will be triggered by the self generated zerocrossing pulse.

III. Design of the firing circuit

The proposed firing circuit has been designed, synthesized, and simulated using Altera Quartus software package. It provides a complete design environment for system-on-programmable-chip (SOPC) design. The package offers a very rich library of parameterized modules (LPM) that can be utilized to construct most of the various counters and sequential circuits used in this design. The schematic (Block) editor is used to desribe the design subsystems as modules. The complete design has been designed and synthesized around FPGA chip. FPGAs are platforms that can be used to design a specific hardware optimized to implement specific digital circuits. Thay are considered to be uncommitted 'sea of logic gates" that can be programmed by connecting the logic gates together to form ant desired digital component such as registers, counters, arithmetic logic units, and so foth. They have a significant advantage of being reconfigurable directly by the software. This adds flexibility in designing the hardware and updating its structure. The programmability, flexibility, prformance, and potential for lower cost have opened up new avenues for FPGAs to be used in a broad range of applicatopns[5].

The time simulation option offered by the software package is a powerful tool for testing and evaluating the logical and arithmetic operations and the limitations for internal timing of the design. It enables the designer to verify the system performance before it is actually committed to real hardware. In fact, it reduces the time required to transform the initial design concept into working silicon drastically. The proposed firing circuit is designed as individual sub-modules in a hierarchal manner which enables the designer to test the various units individually. The Quartus software package provided by Altera is used to design and simulate the proposed firing circuit. The design has been implemented around MAX II PLD chip (EPM1270F256C5 device) [6].

IV. Experimental test

A low cost simple development board included with the MAX II development kit (EZ1CUSB) based on the EPM1270F256C5 device is used. It is a ROM-based (non-volatile) full- featured platform for prototyping and evaluating designs based on programmable logic devices. It operates by 66 MHz clock and the configuration programs can be down loaded from the PC via JTAG interface and parallel port [7].

The prototype set up for the proposed scheme of the firing circuit has been implemented, verified and tested. Fig.3 (a) and (b) shows the display output for the logic analyzer for the firing pulses generated for positive and negative cycles of the three phases when α equal to 115° and 22° respectively.

V. Conclusion

In this paper, a novel configurable hardware implementation single chip firing circuit firing circuit for three phase motor speed control based on (FPGA) hardware architecture is presented. The system has the advantages of being simple, and flexible with built-in self test and low development cost. The performance of the prototype hardware set up proved the concept of the proposed circuit. The system is implemented using MAX II FPGA chip. This programmable hardware environment will give the design the possibility to be applied for further applications.

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Fig.3 Logic analyzer output p of the firing pulses

(a) $\alpha = 115^{\circ}$ (b) $\alpha = 22^{\circ}$

EFFICIENCY AND CONVERGENCE OF THE WAVE CONCEPT ITERATIVE PROCEDURE

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Wave Concept Iterative Procedure, iterative methods

ABSTRACT

In some electromagnetic iterative methods, the convergence to the solution is slow and the stable solution is not always found. The present paper describes three methods used to improve the speed and the stability of the convergence process for the Wave Concept Iterative Procedure (WCIP). Two of these methods are not directly related to the electromagnetic fields computation and can be used in other iterative computing procedures as well.

I. INTRODUCTION

In (Azizi et al. 1995; Azizi et al. 1996) the Fast Wave Concept Iterative Process (FWCIP) is introduced. It relies on the definition of transverse waves based on the tangential electric and magnetic fields on some active surface. The same (essentially) method is denoted in literature as FWCIP (Azizi et al. 1995), Transverse Wave Formulation - TWF (Wane et al. 2005) and more recently Wave Concept Iterative Procedure - WCIP (Baudrand et al. 2007, Raveu et. al 2007).

WCIP compares favorably (Wane and Bajon 2006) with other commercially available software regarding the precision and promises better performance in computation efficiency in structures with very different layer heights.



Figure 1: Wave Concept Iterative Procedure Definitions

Let Ω be a discontinuity plane inside a metallic box (figure 1). The regions on both sides are filled with homogenous dielectric. The two regions are designated as region 1 (ε_{r1} , h_1 , etc.) and region 2 (ε_{r2} , h_2 , etc.).

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Let Ω_i be a surface infinitely close to Ω in region i, n_i the unit vector normal to Ω and directed into region i, i = 1 or 2.

We define the transverse incident and reflected wave in $\Omega_i(1)$:

$$\vec{A} = \frac{1}{2\sqrt{Z_{0i}}} \left(\vec{E} + Z_{0i} \vec{J} \right), \ \vec{B} = \frac{1}{2\sqrt{Z_{0i}}} \left(\vec{E} - Z_{0i} \vec{J} \right)$$
(1)

The waves are subject to constraints imposed by the discontinuity (2) and by the reflection over the metallic walls of the box (3).

$$\vec{A} = \hat{\Gamma}_{\Omega}\vec{B} + \vec{A}_0 \tag{2}$$

$$\vec{B} = \hat{\Gamma}\vec{A} \tag{3}$$

 A_0 is the incident wave generated by the source in the two regions and $\hat{\Gamma}_{\Omega}$, $\hat{\Gamma}$ denotes the reflection operator on the discontinuity surface Ω and on the metallic walls respectively. The WCIP method solves (2) (3) by an iterative procedure. In (4), (5) *k* denotes the current iteration and the starting conditions are imposed by the source (6).

$$\vec{A}^{(k+1)} = \hat{\Gamma}_{\Omega} \vec{B}^{(k)} + \vec{A}_{0} \tag{4}$$

$$\vec{B}^{(k)} = \hat{\Gamma} \vec{A}^{(k)} \tag{5}$$

$$\vec{A}^{(0)} = \vec{A}_0 \tag{6}$$

Equation (2) is applied in the space domain, while (3) is easily implemented in the modal domain, so a fast modal transform (FMT), based on FFT (N'gongo and Baudrand 1999), can be developed in order to go from (4) to (5) and vice versa through the iterative procedure.

While this method found its best applications in the analysis of microwave multilayer structures (Akatimagool et al. 2001, Wane et al. 2005, Wane and Bajon 2006), it has been also successfully applied to cylinders (Raveu et al. 2004) and photonics (Azizi et al. 2008)

The WCIP has some convergence problems, even in simplest structures. In the following example, we show the results found for a microstrip transmission line, extending from one side of the box to another. The box

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is rectangular (a by b), divided by a uniform grid in 32 by 32 pixels. The dimensions are: a = 17mm; b = 17mm; $\epsilon_{r1} = 1$; $h_1 = 1000$ mm; $\epsilon_{r2} = 10$; $h_2 = 1.5$ mm. The line is 2 pixels wide (1.06mm) (figure 1) and of course short-circuited at the end by the box, so purely imaginary impedance is expected. The convergence is verified by plotting the impedance value on the source surface (figure 2).

Figure 2 show that 150 iterations are required to obtain the "convergence" but some big enough oscillations still remain, for the real part around 0, for the imaginary part around -170Ω . These curves show that a real convergence is not reached in 400 iterations and will not be reached, even with more iterations, thus the used algorithm suffers from certain instability. Figure 3 shows the computed fields on the discontinuity plane. The shape of the y direction current J_y clearly shows the instability. Investigation of other fields through the iterations shows little variation in shape and values.



Figure 2: Input Impedance - Convergence Analysis



Figure 3: Original WCIP fields: E_x , E_y (up), J_x , J_y (down)

II. ITERATIVE PROCEDURE IMPROVEMENT TECHNIQUES

We will model the WCIP iterative numerical problem as a discrete in time system. We have an input (the source) and an output: the variation in "time" (read iterations) of the desired quantities (field values, impedances etc.). We will be able to use systems theory in order to insure the WCIP convergence (discrete in time system stability) as in (Smith 1999). As shown in figure 4 we obtain a feedback discrete system, which, as is well known, might have in some cases stability problems.



Figure 4: Iterative Procedure as a Feedback Discrete System

Source modification technique

A step variation source as in (6) will excite high "frequency" oscillations in the solution. A source with a slow variation in time (measured in iterations) will

eventually solve the instability problem, thus offering the desired convergence. From spectral windowing techniques (Nuttall 1981; Lyons 1998), we choose a Blackman-Harris window for its reduced high frequencies contents, decreasing the amplitude of the oscillations.

$$\vec{A}_{0}^{(k)} = \begin{cases} \left[a_{0} + a_{1} \cos\left(\frac{\pi k}{k_{0}}\right) + a_{2} \cos\left(\frac{2\pi k}{k_{0}}\right) + a_{3} \cos\left(\frac{3\pi k}{k_{0}}\right) \right] \cdot \vec{A}_{0}; & k \le k_{0} \\ \vec{A}_{0}; & k > k_{0} \end{cases}$$

$$\begin{cases} a_{0} = 0.3558; a_{1} = -0.4874; \\ a_{2} = 0.1442; a_{3} = -0.0126; \end{cases}$$
(8)

As in (7) with optimal parameters in (8), we increase the source gradually for k_0 iterations before reaching the desired value A_0 . Figure 5 shows the results. In both cases, the final value is almost the same, and we decrease the oscillations. The effect is more obvious for larger k_0 (b) with the expense of the convergence rate. Larger k_0 means lower high frequency content in the source, which implies as we see lower oscillations in the response. Figure 6 shows the fields on the discontinuity plane. The amplitude of the tangential line current is the smallest, so where only noise (oscillations) appeared before in figure 3 now we have a distinct (modal) shape in figure 6. The tangential current in the line is very small but not zero, as we defined the unknown fields in the middle of the pixel. A closer inspection of all the fields show "cleaner" shapes for all the other fields (longitudinal electric field shown in figure 6): the smaller oscillations in the convergence curve imply smaller oscillations in all the field values.



Figure 5: Blackman-Harris Source a) $k_0 = 50$; b) $k_0 = 200$



Figure 6: Blackmann-Harris Source/Modified Structure Fields: E_x, E_y (up), J_x, J_y (down).

Structure modification technique

Another approach is to modify the surface reflection operator. In (4) the surface reflection takes different values for the metal, dielectric and surface impedance. To ensure a smoother convergence we will try to make a soft transition between the different materials, at least until the field reaches a "good enough" value, after which we can return to the physics related surface reflection in order to obtain the correct solution.

We will adopt definition (9) for the surface reflection operator:

$$\hat{\Gamma}_{\Omega}^{(S)} = \alpha(k) \cdot \hat{\Gamma}_{\Omega}^{(S)} + [1 - \alpha(k)] \cdot \frac{\hat{\Gamma}_{\Omega}^{(M)} + \hat{\Gamma}_{\Omega}^{(D)}}{2}$$
(9)

The transition function α will increase gradually from 0 to 1 in k_0 iterations in order to obtain a smooth transition. $\hat{\Gamma}_{\Omega}^{(S)}$ (S - denotes the surface type: D=dielectric, M=metal, Z=surface impedance) will gradually change from the first iterations when we have a homogenous discontinuity (no transition between materials), to the correct values for the surface reflection in k_0 iterations. Various functions can be used but the experience shows that a suitable function must raise fast enough after k=0 in order to improve the convergence rate and also to have a slow variation when approaching k_0 to prevent oscillations. We use function (10) with different values for n to obtain fast convergence and low oscillations.



Figure 7: Modified Surface Reflection, n = 8. a) $k_0 = 50; b$) $k_0 = 200$

Figure 7 shows the results obtained for the same test structure, using the transition function (10) for n = 8. The final fields are identical to those in figure 6 and will not be plotted again. The conclusions are similar to those from the Blackman-Harris source: larger k_0 decrease the oscillations but increase the convergence time while the *n* parameter has an opposite effect.

III. MODIFIED WAVE DEFINITION

In the previous section, we investigated two methods that can be used in any iterative procedure to improve the convergence, but those methods, while offering a better convergence and a better field solution, only lowers the intrinsic instability of the WCIP method.

Some changes are to be made inside the method itself. In WCIP many of the concepts are physics related and cannot be changed. The only place where we imposed some of the parameters is the definition of the waves where we chose a space domain definition (1). The value of the impedance was chosen equal to that of the corresponding medium (11).

$$Z_{0i} = \sqrt{\frac{\mu_0}{\varepsilon_i}} , \forall i = 1,2$$
(11)

This value is not imposed by any physical constraints so in principle it can be changed. This approach has not shown an improvement in the convergence procedure so it seems that the only adjustable parameter will not give us the means to stabilize the system.

Modal domain definition of the waves

We will try to define the waves in the modal domain. For every region, we state the modal decomposition:

$$\begin{cases}
A_{mn} = \frac{1}{2\sqrt{Z_{0mn}}} (V_{mn} + Z_{0mn} \cdot I_{mn}) \\
B_{mn} = \frac{1}{2\sqrt{Z_{0mn}}} (V_{mn} - Z_{0mn} \cdot I_{mn}) \\
\vec{A} = \sum_{mn} A_{mn} f_{mn} ; \quad \vec{B} = \sum_{mn} B_{mn} f_{mn} \\
\vec{E} = \sum_{mn} V_{mn} f_{mn} ; \quad \vec{J} = \sum_{mn} I_{mn} f_{mn}
\end{cases}$$
(12)

where: $i = \overline{1, M}$; $j = \overline{1, N}$; $M = 2^m$; $N = 2^n$ and Z_0 becomes a matrix resulting in a different impedance value for every spatial mode: Z_{0mn} .

As seen from (4) the surface reflection operator needed in order to apply WCIP is localized so cannot be conceived in modal domain and its value relies on a constant value of the impedance. As a first impression, definitions (12)-(13) are not possible. We can yet find a method to decouple the modes. First, we write the iterative procedure from (4)-(6):

$$\vec{A}^{(k+1)} = \hat{\Gamma}_{\Omega} \cdot FMT^{-1} \left(\hat{\Gamma} \cdot FMT \left(\vec{A}^{(k)} \right) \right) + \vec{A}_{0} \qquad (14)$$

The surface reflection operator takes different values depending on the surface type.

$$\hat{\Gamma}_{\Omega}(x, y) = H_M(x, y) \cdot \hat{\Gamma}_{\Omega}^{(M)} + H_D(x, y) \cdot \hat{\Gamma}_{\Omega}^{(D)} + H_Z(x, y) \cdot \hat{\Gamma}_{\Omega}^{(Z)}$$
(15)

$$H_M(x, y) = \begin{cases} 1 & \text{on the metal} \\ 0 & \text{elsewhere} \end{cases}$$
(16)

In the same way as in (16) we define the localization function for the dielectric and for the lossy dielectric.

We can see that the spatial variables x and y appear only in the localization functions and not in the specific surface operator. Thus, we can move these operators inside the Inverse FMT, in fact moving the surface reflection in the modal domain.

$$\vec{A}^{(k+1)} = H_M(x, y) \cdot \vec{A}_M^{(k)} + H_D(x, y) \cdot \vec{A}_D^{(k)}$$

$$+ H_M(x, y) \cdot \vec{A}_M^{(k)} + \vec{A}$$
(17)

$$\vec{A}_{\mathcal{M}}^{(k)} = \hat{\Gamma}_{\mathcal{O}}^{(M)} \cdot FMT^{-1} \left(\hat{\Gamma} \cdot FMT^{\left(\vec{A}^{(k)} \right)} \right)$$
(18)

$$\vec{\boldsymbol{\lambda}}_{M}^{(k)} = \hat{\boldsymbol{\Gamma}}_{M}^{(D)} \cdot \boldsymbol{\boldsymbol{F}} \boldsymbol{\boldsymbol{M}} \boldsymbol{\boldsymbol{T}}^{-1} \left(\hat{\boldsymbol{\Gamma}} \cdot \boldsymbol{\boldsymbol{F}} \boldsymbol{\boldsymbol{M}} \boldsymbol{\boldsymbol{T}} \left(\vec{\boldsymbol{A}}^{(k)} \right) \right)$$
(19)

$$\vec{A}_{C}^{(k)} = \hat{\Gamma}_{C}^{(Z)} \cdot FMT^{-1} \left(\hat{\Gamma} \cdot FMT \left(\vec{A}^{(k)} \right) \right)$$
(20)

We find every particular solution (18)-(20) with the hypothesis that the discontinuity plane is homogenous: all metallic (18) or all dielectric (19) or all lossy dielectric (20). Then we find the correct solution (17) choosing for every pixel in the grid the corresponding value.

This method allows now the existence of $2 \times M \times N$ parameters which we can modify in order to improve the convergence speed and the stability of the solution. Some tests have been carried out to prove the validity of the theory and the method works fine for Z_{0mn} defined as in (11). We obtain exactly the same results as before.

Edge effect

We must find the right strategy to define the spatial mode impedance Z_{0mn} . Figure 2 show the existence of some instability that we believe to be connected to the spatial distribution of the electromagnetic fields, especially in the vicinity of the metal - dielectric transition (Wane et al. 2005).

It is probably necessary to explain the above statement. Let us look to the field distributions found by the "classic" WCIP method. The structure is the same microstrip line used before, placed in the middle of the box, along the x axis. The frequency is set to 5GHz. The line being only 2 pixels wide we expect only longitudinal current to exist on the line. Even incomplete as stated before and with errors, WCIP offers still the "good" shape of the fields (Edwards 1992; Gupta et al. 1996). As in figure 8 only E_y and J_x have considerable values, while E_x and J_y are small and "noisy", and appear as an influence of the source (which creates x direction fields) and mainly due to method errors (the lack of the convergence).



Figure 8: Transversal Field (E_y) and Longitudinal Surface Current (J_x)

Figure 8 shows two interesting facts. First, the E_y and J_x fields seem connected and in antiphase. We will investigate this connection later. Second and more important, both E_y and J_x , and consequently the waves A_x , A_y , B_x , B_y (as E_x and J_y can be neglected) have some major step discontinuities when going through a dielectric-metal discontinuity. These step discontinuities will not be accurately modeled by complex exponentials (as in the Fourier transform or even in the general TE/TM modes theory). It is our belief that this fact generates the instability of the WCIP method.

Let us consider a dielectric-metal interface along the xaxis as in figure 9. We consider a metallic sheet, occupying the x>0 semi plane in the xOy plane. The sheet height will be considered to be 0 (dz \rightarrow 0) for the case of the ideal planar circuit, and the width of the sheet analyzed will be decreased (dy \rightarrow 0) for the investigation of the edge effect (distribution of the fields around the Ox axis).



Figure 9: Edge Effect on an X Axis Discontinuity

On the metal-dielectric interface, the fields are described by:

$$\vec{n} \cdot \vec{D} = \rho_S; \ \vec{n} \cdot \vec{B} = 0; \ \vec{n} \times \vec{E} = 0; \ \vec{n} \times \vec{H} = \vec{J}_S \ (21)$$

We apply (21) on two dielectric-metal interfaces, denoted by the normal vectors n_1 and n_2 .

$$D_{1z} = \rho_{S1}; H_{1z} = 0; E_{1x} = E_{1y} = 0;$$

$$H_{1y} = -J_{S1x}; H_{1x} = J_{S1y}$$
(22)

If we consider the edge effect, we apply (22) in the proximity of the interface $(dy\rightarrow 0)$ so the normal surface current (J_{Sy}) becomes 0, the surface current distribution changes to a linear distribution and, correspondingly, the surface charge density transforms into a linear charge density, along the edge: ρ_x .

Therefore, for $x \approx 0$; x > 0, the following apply:

$$E_{1x} = E_{1y} = H_{1z} = H_{1x} = 0$$

$$D_{1z} = \rho_x \cdot \delta(y), H_{1y} = -J_{S1x}$$
(23)

For the second interface, we find in the same way for $x \approx 0$; x < 0:

$$E_{2x} = E_{2z} = H_{2z} = H_{2y} = 0$$

$$D_{2y} = -\rho_x \cdot \delta(z); H_{2z} = -J_{S2x}$$
(24)

We must find the connection between the linear current density J_{Lx} and the linear charge density ρ_x . To achieve this we will consider an elementary volume on the interface between the metal and the dielectric like in figure 10.



Figure 10: Charge Conservation in an Elementary Volume.

The calculus of the charge conservation in the elementary volume and equations (23) and (24) offer the connection between the fields existing in each side of the x-axis metal-dielectric interface:

$$\frac{\partial J_x}{\partial x} = -j\omega\varepsilon \cdot E_y \tag{25}$$

Correspondingly, for the dielectric-metal interface along the y-axis we obtain:

$$\frac{\partial J_y}{\partial y} = -j\omega\varepsilon \cdot E_x \tag{26}$$

Redefinition of the waves

From (25) and (26) we can see that there is a definition of the wave functions that will allow a smooth transition over the metal-dielectric interfaces. In the space domain this definition will be:

$$\vec{A} = \vec{E} - \frac{1}{j\omega\varepsilon} \cdot [R] \cdot \nabla \vec{J}$$
(27)

$$\vec{B} = \vec{E} + \frac{1}{j\omega\varepsilon} \cdot [R] \cdot \nabla \vec{J}$$
(28)

where [R] is a rotation operator that interchanges the x and y components of a vector (29).

$$\begin{bmatrix} R \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$
(29)

Definitions (27) and (28) allow the extraction of the electric field, but the surface current can be obtained only by integration of the divergence operator. Like in section 2 we will try to define the waves in the modal domain. Some problems arise and must be solved.

First, the x and y components of a vector have different basis functions. In all the methods described above, x and y where independent directions and where treated separately the only connection between the two directions was made through a separation transform \tilde{K} but after the modal decomposition. Definitions (27) and (28) rely upon a mixture between x and y components and we must find a way to do this before the modal decomposition.

Both x and y components of $\nabla \vec{J}$ have a harmonic surface decomposition after the basis functions $h_{mn} = \sin \frac{m\pi x}{a} \cdot \sin \frac{n\pi y}{b}$ and cannot be added with E_x and E_y maintaining the possibility of the modal decomposition after the basis functions (30). In order to preserve the classic definition of the TE/TM modal decomposition we define the waves in the modal domain as in (31).

$$\begin{cases} f_{mn} = \cos \frac{m\pi x}{a} \cdot \sin \frac{n\pi y}{b}; (x \ direction) \\ g_{mn} = \sin \frac{m\pi x}{a} \cdot \cos \frac{n\pi y}{b}; (y \ direction) \end{cases}$$

$$\begin{cases} A_x = E_x + \hat{Z}_0^x \cdot \sum_{mn} \langle J_y, g_{mn} \rangle \cdot \langle f_{mn} | \\ A_y = E_y + \hat{Z}_0^y \cdot \sum_{mn} \langle J_x, f_{mn} \rangle \cdot \langle g_{mn} | \end{cases}$$

$$(30)$$

In fact, in (31) an intermediary function with no physical correspondent is defined and the surface current is replaced by a composition of the modal amplitudes by a rotated modal basis. Equations (31) do not accurately apply (25) and (26) but with the appropriate choice of the impedance coefficients, we

can make the transition over different materials as smooth as possible.

We apply (31) with the following impedance coefficients:

$$Z_{mn}^{x} = -\frac{n\pi}{j\omega\varepsilon \cdot b}, \quad Z_{mn}^{y} = -\frac{m\pi}{j\omega\varepsilon \cdot a}$$
(32)

The convergence plot for the same structure as in section 1 is in figure 11. This time the input impedance computed from the redefined waves (31) loses its physical sense as we perform the inversion of these definitions only at the end of the iterative procedure, but it is an accurate description of the convergence towards the solution.



Figure 11: Convergence Analysis - New Definition

IV. CONCLUSIONS

We present in this work three methods used to improve the convergence efficiency in WCIP. All computations were performed using custom software developped in our laboratory in C++ and visual Windows technology.

Section II introduces two generally available methods, appropriate for almost any iterative methods. Analogy with a discrete in time feedback system allows altering temporarily the energy source and/or the structure itself in order to achieve better convergence. We obtain more accurate and faster results in term of field distributions. Relative improvement in speed is between 2 and 3 depending on the parameters of the alteration, with the added benefit of the improved solution.

Section III offers a particular method in the case of the WCIP. We obtain a very good behavior of the iterative procedure. The new definition of the waves reaches a stable solution in around 30 iterations as opposed to 150 iterations in figure 2 and without the oscillations showing the lack of convergence of the classic method.

This work is still in progress. Alternate definitions of the impedance matrices in (31) are investigated, in order to provide a smooth transition of the waves over the metal/dielectric edge.

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INVESTIGATION OF THE HEXACHIRAL HONEYCOMB EMC PROPERTIES BY FULL WAVE ELECTROMAGNETIC SIMULATION

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ABSTRACT

A hexachiral honeycomb structure with good mechanical properties, is investigated through full wave electromagnetic simulation. This new material shows some interesting EMC properties and promises better performance using different insertion techniques. The effect of the electromagnetic chirality is investigated. Design maps and thermal computations are derived.

I. INTRODUCTION

In the past years, an increasing amount of effort has been invested in the development of new materials, with good mechanical properties, low weight and low cost. In particular auxetic materials benefit from their negative Poisson's ratio (Grima 2007) and are investigated closely in the last decade (Li et al. 2000, Ammari et al. 1998, Oussaid R. and Haraoubia B. 2004). In the same time, we witness an increased utilization of the RF spectrum, especially in the free bands (2.4GHz). Coding techniques have been developed to ensure the "peaceful" coexistence of multiple emitter/receiver pairs in the same frequency band. In some cases, these techniques are not sufficient, especially when good shielding for an enclosure is imperative (aeronautics - Bornengo D. et al. 2005, medicine etc.). A natural step forward is to investigate the electromagnetic properties of these materials, in order to provide good electromagnetic shielding.

Electromagnetic metamaterials are defined as artificial effectively homogeneous electromagnetic structures with unusual properties not readily available in nature. An effectively homogeneous structure is a structure whose structural average cell size *L* is much smaller than the guided wavelength λ_g . i.e. the average cell size should be at least smaller than a quarter of wavelength (Caloz and Itoh 2006),

$$L < \frac{\lambda_g}{4} \tag{1}$$

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) The condition (1) is known as the effectivehomogeneity limit or effective-homogeneity condition, and ensures that refractive phenomena will dominate over scattering/diffraction phenomena when a wave propagates inside the medium. In the present application, the frequency range of interest (1 to 15GHz) implies a guided waveguide between 10 mm and 150 mm, and we expect the chirality defined by geometry to play an electromagnetic role, depending on the cell size, especially at higher frequencies (7 to 15 GHz).

Depending on the method used for defining the magnetoelectric dyadics, there are multiple constitutive relations in extensive use for chiral mediums: Drude-Born-Fedorov (Athanasiadis and Costakis 2000, Oksanen et al. 1992) Post (Jaggard et al. 1988), Tellegen (Qiu et al. 2007). Equivalence between these relations can be obtained (Liu and Li 1999) by substitution in Maxwell's equations.

Widely used are Post constitutive relations in the frequency domain, valid for time harmonic electromagnetic fields: Eqs. (2), (3).

$$\mathbf{D} = \varepsilon_c \mathbf{E} + j \xi_c \mathbf{B} \tag{2}$$

$$\mathbf{H} = j\xi_c \mathbf{E} + \mathbf{B}/\mu_c \tag{3}$$

where ε_c and μ_c represent an equivalent of the permittivity and permeability, ξ_c the chirality admittance, which is a measure of the handedness of the medium and j is the imaginary unit.

II. SIMULATION SETUP

The structure used in tests was a fiber reinforced polymer prototype, developed in the framework of the CHISMACOMB (CHIral SMArt honeyCOMB) FP6-EU-013641 project (Chismacomb 2008), by Italcompany (figure 1). The structure is a hexachiral honeycomb, each of the equally spaced cylinders being connected to his 6 neighbors by ligaments and is based on the idea found in (Prall and Lakes 1997) which is a simplification of a two-dimensional molecular model studied earlier (Wojciechowski 1989).



Figure 1: Rectangular Unit Cell.

The interaction between a plane wave and an infinitely large sheet of auxetic material at normal incidence was investigated. The boundary conditions were set to electric wall (both walls on x directions) and magnetic wall (y direction walls). An input wave port was placed at a distance equal to the minimum between the 8th part of the wavelength and 5 mesh lines from the structure, the second (exit) wave port is added only when losses inside the structure were taken into account.

In order to limit the model's dimensions, the periodicity of the structure was investigated. While the intrinsic unit cell for this structure will contain only one cylinder and half of every surrounding ligament, numerical electromagnetic computation demands a rectangular unit cell which can be placed on a regular (not staggered) rectangular grid in order to preserve electromagnetic fields symmetries. The rectangular unit cell is showed in figure 2, the length and width being equal to $W = 2 \cdot L$ (x direction) and $H = L \cdot \sqrt{3}$ (y direction) respectively (where L is the cylinder separation). Table 1 shows the typical dimensions used in tests when we parameterize the others.

Parameter	Description	Value
D	Internal cylinder diameter	18.58 mm
L	Cylinder separation	24.72 mm
h	Height of the panel	19.75 mm
g	Ligament width	3.3 mm
ε _r	Electrical permittivity	2.5 (4)
tan δ	$\tan \delta$ Loss angle tangent	

Table 1: Typical Dimensions.

The results of the simulations show the S parameters for the structure. The typical shielding parameters reflectance, transmittance and absorption are related to the S parameters by the following equations (Hong et al. 2003), as long as the surrounding medium is lossless:

$$R = \left| S_{11} \right|^2 \tag{4}$$

$$T = |S_{21}|^2$$
 (5)

$$=1-R-T=1-\left|S_{11}\right|^{2}-\left|S_{21}\right|^{2}$$
 (6)

III. ACCURACY OF THE RESULTS

A

The CST Microwave Studio frequency domain solver solves the problem for a single frequency at a time, and for a number of adaptively chosen frequency samples in the course of a frequency sweep. For each frequency sample, the linear equation system will be solved by an iterative (e.g. conjugate gradient) or sparse direct solver.

The CST Microwave Studio time domain solver calculates the development of fields through time at discrete locations and at discrete time samples. It calculates the transmission of energy between various ports and/or open space of the investigated structure.

For the hexachiral structure under test, the auxetic layer is illuminated with a plane wave, coming from the z direction, with normal incidence to the material. The polarization of the plane wave in the material is imposed by the electric/magnetic wall boundary conditions, and for correct calculations we expect the electromagnetic fields inside the structure to follow the characteristics of the incident wave. As in figure 2, we find that inside the hexachiral honeycomb, the electric field will have only E_x component, whereas the magnetic field shows only H_y component.

The final test was the comparison between the FDTD and FDFD analysis results for the same structure. The two computation methods are not related, even the mesh is different in this case (hexahedral with Perfect Boundary Approximation[®] - PBA for FDTD and tetrahedral for the frequency domain solver). The results are found to be essentially the same (see figure 3).

The difference between the two curves is maximum ± 1 dB in the 1 $\div 10$ GHz range, except the frequencies around the reflection annulment, where a slight variation of the zero's frequency is detected (0.1GHz, meaning a 1.8% difference between the two minima) around 5.8GHz. The two solvers are independent even if they belong to the same software suite, so we can estimate a ± 2 dB general error coupled with a $\pm 2\%$ peak detection error for the rest of the simulations.



Figure 2: E_x (left) and H_y (right) Inside the Structure



Figure 3: S₁₁ for the Loseless Structure by FDFD (left) and FDTD (right) Computation

IV. RESULTS AND INFLUENCE OF CHIRALITY

Parametric studies investigated the effect of the dimensions (L, D, h, g) and material properties (ε , σ , tan δ). Figure 4 shows the influence of L, h (in this order) for the lossless dielectric over the reflection coefficient (S₁₁), and figure 5 shows the influence of ε and tan δ over reflection coefficient (S₁₁) or over the transmission coefficient (S₂₁) when losses are taken into account

Analysis shows that the chiral structure has almost identical properties (figures 4, 5) with an equivalent homogenous dielectric layer, so the mechanical and thermal advantages provided by the structure do not affect the electromagnetic properties in the bandwidth considered (0.1-10 GHz).





Figure 5: Electrical permittivity (ϵ - left) and Loss tangent (tan δ - right) influence over S_{11}/S_{22}

Figures 4-5 show that for the lossless chiral layer we have a typical half-wave reflectionless slab (Orfanidis 2008). We obtain zeroes for the reflection coefficient at the frequencies that verify the condition:

$$h = k \cdot \frac{\lambda_g}{2} = \frac{k}{2} \cdot \frac{c}{f \sqrt{\varepsilon_{eff}}} \tag{7}$$

where k must be an integer and λ_g is the guided wavelength, inside the equivalent homogenous dielectric slab. This behavior offers interesting electromagnetic applications, as radar invisibility or building wall transparency.

Equation (7) offers the possibility to use the results in figure 4 to investigate the variation of the effective electrical permittivity on the frequency. Every value for layer's height (h) generate at least two minima of the reflectivity in the bandwidth considered, corresponding to k=1, k=2 in equation (7). We can compute the effective electrical permittivity with equation (8).

$$\varepsilon_{eff}\left(f_{\min,k}\right) = \left(\frac{k \cdot c}{2f_{\min,k} \cdot h}\right)^2 \tag{8}$$



Figure 6. Effective electrical permittivity

The effective electrical permittivity increases linearly with the frequency, as the electromagnetic field is confined inside the dielectric at higher frequency. The results in figure 4 on which figure 6 is based are obtained for $\varepsilon = 2.5$ for the base material. In this case, we find the effective permittivity ranging from 1.61 to 2.1, depending on the frequency. In addition, as the frequency increases we notice slight variations from the predicted linear increase, as the chirality of the structure becomes more and more evident.

The effects of the chirality appear as we increase the frequency, the electrical permittivity and the cylinder separation. In the typical situation (table 1), equation (1) gives a frequency limit of about 2.37 GHz. Close inspection of the results (figure 4) shows that obvious effects of the microscopic chiral structure are visible at 8 GHz.

Condition (1) can be expressed in terms of visible influence as:

$$L \cdot f \cdot \sqrt{\varepsilon_{eff}} \approx \frac{3c}{4} \tag{9}$$

The other results verify this relationship. Increase of ε from 2.5 to 10 (figure 5) lower the frequency of appearance of chiral effects from 8GHz to 4 GHz (the square root of the permittivity factor of 4). Increase of L to 40 mm (figure 4) show the same effect starting from 5GHz.

We can conclude that regarding the hexachiral honeycomb, chirality influence becomes obvious when relation (9) applies, but while visible, this influence does not affect the macroscopic behavior of the panel under test. The hexachiral panel behaves as a homogenous dielectric, with a different effective electrical permittivity (figure 6).

V. PARAMETRIC ANALYSIS AND DESIGN MAPS

The results in figures 4, 5 offer important information regarding the behavior of the intrinsic chiral panel but are less suggestive from a macroscopic or "application" point of view. The macroscopic values of interest for a microwave shield designer are generally related to transmittance (figure 5b) at some critical frequencies (typically 0.9÷1GHz - the GSM band, 2.4 GHz - free use frequency bandwidth, and 5.8 GHz – a second free bandwidth) or reflectivity parameters (figures. 4-5a) as the frequency of the first minimum, the out of band maximum reflectivity (first and second maximum), depending on the application.

The question a designer is asked is rather an "inverse" of the answer from figures 4, 5. Usually the designer is not interested by the performance of "that" material, but instead the question is: "what material must I choose to obtain a certain transmittance or a certain reflectivity". In the next set of analyses, the aim is to investigate the influence of the material properties (tan δ and ϵ) over the transmission and reflectivity properties.

Table 2: Geometric Parameters Sweep.

Parameter	Range	Step
D	20÷50 mm	5 mm
Н	20÷50 mm	5 mm
L/D	1.5÷3	0.25
D/g	5÷20	2.5

In the first set of computations we maintain the same geometrical properties (D, L, h, g - Table 1) but we insert variations in material properties: $\tan \delta = [0, 0.5]$ and $\varepsilon = [1.5, 10]$. S₁₁ and S₂₁ are computed. The parametric curves are plotted in figure 7 in order to facilitate shielding design with the hexachiral honeycomb. We represent the transmittance at the three

selected frequencies and the minima/maxima of the reflectance.

For the second set of computations we choose L/D and

and with fixed dielectric parameters ($\varepsilon = 4$ and tan $\delta =$ 0.01) we make the transmission and reflection computation for geometric parameters as in Table 2. The results are plotted in figure 8.

18-20

16-18

14-16

12-14

10-12

8-10

6-8

4-6

2-4

■ 0-2

20-21

19-20

<mark>=</mark> 18-19

17-18

16-17

15-16

14-15

13-14

12-13

11-12

10-11

9-10

8-9

11.3-12
 11-11.5
 10.5-11
 10-10.5

9.5-10

9-9.5

9-9.5
8.5-9
8-8.5
7.5-8

7-7.5

■ 6.5-7 ■ 6-6.5

5.5-6

5-5.5

■ 4.5-5 ■ 4-4.5

3 5-4

7 8 9 10

6

5 7 9 10 ■ 7-8

5 6 78 9 10 3-3-4

epsilon

epsilon

6 8



Figure 7 Dielectric Properties Design Maps.

4.1-4.2











Figure 10: Power Loss Density at 10.69GHz

VI. THERMAL DISTRIBUTION

Simulations have been performed in order to identify the energy absorption characteristics inside the material. The first results emphasize an energy concentration depending solely on the hexachiral geometry. The power loss density inside the ligaments of the hexachiral honeycomb is an indication of energy dissipation inside the structure. The two frequencies are chosen. 3.06GHz and 10.69GHz those corresponding to a minimum of the reflectance (figure 9) and transmittance (figure 10) respectively, as the frequencies at which maximum thermal effect is expected.

A concentration of the energy dissipation will generate a temperature increase in certain points. However, this energy is not accumulated, the most significant heat transfer mechanism being thermal conduction (eq. 7). The speed of the heat transfer through a portion of material of transversal area A and length x depends on the steady state temperature difference.

Heat is generated differently in two points according to the electromagnetic energy concentration pattern (eq. 5). We can estimate the steady state for the thermal phenomenon when the difference between the generated heat in every point equals the heat transferred by conduction between the same points (eqs. 10-11).

$$\Delta \left(\frac{dQ}{dt}\right) = \frac{dQ}{dt}\Big|_{1} - \frac{dQ}{dt}\Big|_{2} = \Delta P_{V} \cdot dV$$
(10)

$$\left. \frac{dQ}{dt} \right|_{1-2} = k \cdot A \cdot \frac{\Delta T}{x} \tag{11}$$

We used the same software suite (CST Microwave Studio) described in section IV, with the difference that in single frequency analysis the FDFD (Finite Differences in Frequency Domain) solver was used to compute the fields inside the structure. The computation is full 3D, figures 9-10 show the power loss density in different longitudinal sections through the panel.

The power loss distribution is mainly longitudinal (in the direction of the incident wave). The incident illumination is 320W/m² (normalization: 1W over the surface of the input port), a rather high value if we consider that the safety limit for RF workers is $50W/m^2$. While such a situation is not usually encountered, we can use eqs. (10), (11) to estimate the temperature gradient which will appear inside the hexachiral structure. At 3.06 GHz (figure 9), we have maximum $\Delta P_V \approx 12,000 \text{ W/m}^3$ and $\Delta P_V \approx 30,000 \text{ W/m}^3$ inside the cylinder and inside the ligaments respectively. The maximum temperature variation is $\Delta T \approx 4$ K and $\Delta T \approx$ 10 K respectively. As the power losses are related to transmission behavior, we expect greater effect when the transmittance reaches a minimum. At 10.69 GHz (figure 10), we have maximum $\Delta P_V \approx 53,000 \text{ W/m}^3$ and $\Delta P_V \approx 95,000 \text{ W/m}^3$ inside the cylinder and inside the ligaments respectively, the corresponding temperature variation being $\Delta T \approx 18$ K and $\Delta T \approx 33$ K respectively.

In typical applications (10 to 50 W/m² - safety limits) the effect is less important (up to 5K temperature differences) but the differences in temperature can reach 100K at 1kW/m^2 illumination. Wireless Power Transmission can use up to $30 \div 90 \text{ kW/m^2}$ at the space reflectors.

The simple hexachiral panel, subject to localized electromagnetic power dissipation develops thermal gradients which affect the mechanical performance thus thermal analysis in high power applications must rely on temperature gradient instead of uniformity.

CONCLUSIONS

In this paper a complete investigation of the hexachiral honeycomb by full wave electromagnetic simulation is performed. The software suite CST Microwave Studio is used, with the added benefit of the presence of multiple solvers. This allowed us to perform accuracy estimation (secton III) and extended the range of simulations we were able to perform.

The time domain solver (FDTD) was used in those situations where multiple simulations were needed and speed was an important issue (more than 10,000 different individual simulations were performed). Multiple parametric simulations were made, which allowed the investigation of the chirality in section IV and the derivation of the design maps in section V.

The frequency domain solver (FDFD) which is slower but more accurate in small bandwidths was used in order to verify the boundary conditions used (section II) and in order to investigate the microwave power distribution inside the material, which allowed the thermal analysis in section VI.

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A NOVEL CONTROL OF AC VOLTAGE CONTROLLER UNDER **INDUCTION MOTOR LOAD**

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KEYWORDS

FPGA. Induction motor. PSIM. triac. Voltage controller.

ABSTRACT

A novel, simple and reliable digital firing scheme has been implemented for soft starting and speed control of three-phase induction motor using ac voltage controller. The system consists of three-phase supply connected to the three-phase induction motor via three triacs and its control circuit. The ac voltage controller has three modes of operation depending on the shape of supply current. The performance of the induction motor differs in each mode where the speed is directly proportional with firing angle in two modes and inversely in the third one. So, the control system has to detect the current mode of operation to choose the correct order for the firing angle of triacs. Three sensors are used to feed the line currents to control system to detect the mode of operation. The control strategy is implemented using a low cost Xilinx Spartan-3E field programmable gate array (FPGA) device. Three PI-controllers are designed on the FPGA to control the system for the three-modes. Simulation of the system is carried out using PSIM computer program. The simulation results show stable operation for different loading conditions especially in mode 2/3. The simulation results have been compared with the experimental results from laboratory prototype.

INTRODUCTION

Speed control of three-phase induction motor can be achieved by stator voltage variation using three-phase controller. This controller consists of three triacs connected as shown in Figure 1. This system has been used in speed control of three-phase induction motor in many literatures (Lipo, T.A. 1971; Hamed, S. et al.1990; Kamaike, H. 1977 - more references). Although this technique are characterized by low cost, simple and rugged design, it is suffering from many difficulties as high harmonics in the supply currents, narrow speed control range, and different performance depending on the shape of supply currents. The harmonic contents in line currents can be reduced using modern harmonic reduction techniques as active filters or third harmonic injection technique (Ali M. Eltamaly 2008; Bhuvaneswari, G. et. al.). The problem of the different performance depending on the shape of supply currents can be removed using control system that can detect the mode of operation of the system as explained and implemented in this paper. The ac voltage controller has three mode of operation depends on the shape of supply current namely 0/2, 0/2/3, and 2/3 (Lipo, T.A. 1971; I. Alolah et. al. 2006). The best mode of operation is 2/3because of law THD in its line currents, high efficiency and low pulsating torque. To force the motor to work in 2/3 mode of operation, it is required to follow the limits of mode 2/3. The motor speed is directly proportional to the firing angle in modes 0/2 and 0/2/3 and inversely proportional in mode 2/3. So, the control system has to detect the mode of operation to produce the correct firing angle.

COMPUTER SIMULATION

Simulation of three-phase phase ac controller under three-phase induction motor load has been carried out using PSIM 6.1 computer program and SIMULINK to validate the simulation results. The induction motor model in stationary reference frame has been used in the simulation (M. G. Solveson. 2004; M. G. Solveson, B. Mirafzal, and N. A. O. Demerdash, 2006). The details of the simulation of the induction motor and ac voltage controller have been shown in many researches (H. A. Ashour; R.A. Ibrahim, 2007; Gastli,; M. M. Ahmed, 2005; Xu Dianguo; Zhao Kaiqi; Wang Yi. 2003; Rajaji, L.; Kumar, C. 2008; Ali M. Eltamaly 2008° Bhuvaneswari, G.; Charles, S.; Nair, M.G. 2008).

The nameplate motor data used in this simulation is; 1kW, 380 V, Y-connected, 3.0A, 4-pole, 60 Hz, its pu parameters are: $R_s = 0.0583 \,\text{pu}, \quad R_r = 0.0417 \,\text{pu},$ $X_s = 0.125$ pu, $X_r = 0.018$ pu, and $X_m = 1.05$ pu.

Intensive simulation has been carried out for soft starting and speed control at different operating conditions to determine the operating limits of this system. Each mode for different speed and load torque for different firing angle are shown in Figure 2 and Figure 3 respectively. The motor speed is directly proportional with the firing angle in modes 0/2 and 0/2/3 and inversely proportional in mode 2/3 as shown in Figure 4. The system operates in a highly distorts supply current especially in light loads and low firing angle which occurs in modes 0/2 and 0/2/3. So it is better to avoid the operation of the motor in these modes.

The logic used in the design of digital controller is shown in the following sections. Figure 5 shows the main block diagram for the whole control system. This main block diagram has several sub-blocks each one handles a separate function that will be detailed in the following sections.

Zero crossing detector-block receives the square waveform from external zero crossing circuit for each phase voltage. Zero crossing detector blocks generate synchronization pulses to synchronize internal control logic with phase voltages. Sine-wave half cycle counter block generates three digital saw-tooth signals using free running counters with a double of the main supply frequency. Each saw-tooth counter is synchronized with one of phase voltages using zero crossing pulse. The saw-tooth counter is used to represent the value of instantaneous angle of each phase.

DIGITAL CONTROLLER

As explained before the system has to detect the mode of operation to decide to take the suitable action to control the speed. Three PI-controllers should be designed to match the performance of the motor in each mode as shown in Figure 5. The motor speed is measured using speed sensor and fed to ADC to be compared with the reference speed to determine the error signal which is fed to the three PI-controllers as shown in Figure 5. The limits decoder receives the signals from three-phase current sensors to determine the mode of operation of the motor in order to select the correct PI-controller using the control MUX block. The firing angle control block receives the calculated firing angle from the selected PI-controller, clips the firing angle to ensure that the firing angle lies between its maximum and minimum allowable values, and applies this change to current firing angle every new cycle of phase voltage. Angle detection and pulse duration counter block receives the firing angle and the sawtooth counter values to generate three pulses for the three triacs.



Figure 1 Three-phase ac voltage controller under induction motor load.



Figure 2 Limits of each modes for different motor speed.



Figure 3 Limits of each modes for different torque.



Figure 4 Variation of speed with torque and firing angle.



Figure 5 Simplified block diagram of main control system.

Zero Crossing Detector-Block

Zero crossing point is detected by simple logic circuit and an external analog comparator. Zero crossing comparator output is a square waveform has a +V value with the positive half cycle of phase voltage and 0 with the negative half cycle of phase voltage as shown in Figure 6. The required signal for the control system has two pulses for each period one when the comparator output changes from 0 to +V and the other when it changes from +V to 0. The pulse duration is only one FPGA clock cycle. Comparing any two successive samples of comparator output using XOR logic function will generate the pulses whenever the comparator output changed as shown in Figure 6. Comparator output sampled using a single bit register, and the register input and output are applied to XOR logic gate. AND gate and an inverter are used to disable zero crossing pulse generation whenever a global system reset is applied. Each phase has a separate zero-crossing detector block to synchronize the saw-tooth counter with phase's voltages.

B Sine-wave Half Cycle Counter-Block

The output of logic circuit used in sine-wave half cycle counter block is a digital saw-tooth waveform with a frequency of two times the supply frequency. The circuit is a digital accumulator which incremented every positive edge of FPGA core clock and reset whenever it reaches its maximum value or a zero crossing is detected.

In the moment of the saw-tooth waveform reach its maximum, the saw-tooth is reset and starting count from zero for the next half cycle of sinusoidal phase voltage. Resetting the saw-tooth when the phase voltage has a zero cross; grants that the saw-tooth and phase voltage starts from zero value at the same time, this shown in Figure 7. So, the maximum value of saw-tooth waveform can be obtained from (1).

$$C_{\max} = \frac{T}{2*t_c} = \frac{f_c}{2*F}$$
(1)

The angle of the phase voltage equals its frequency times time $\theta = f^*t$. The instantaneous angle value is directly proportional to the time. Also the instantaneous value of saw-tooth is directly proportional to time, this concludes that the instantaneous value of saw-tooth is directly proportional to the instantaneous value of phase angle or $C_i \alpha \theta_i$.

Using the relation between phase angle and saw-tooth instantaneous values, equation (2) can be used to convert any given phase angle to a respective saw-tooth value.

$$C_{\theta} = C_{\max} \frac{\theta}{180} \tag{2}$$

For a chosen firing angle value θ_f , the respective sawtooth value C_{θ} can be obtained from (2) by substituting θ with θ_f . The firing pulse has a finite width of θ_p degrees; this is equivalent to ΔC_{θ} change in saw-tooth value since the firing pulse starts. The value of ΔC_{θ} can be obtained from (2) by substituting θ with θ_p . The values of C_{max} and C_{θ} are rounded to the nearest integer value as the digital control is designed to work with fixed numbers representation only. The relation between phase voltage, saw-tooth waveform, firing pulses and FPGA core clock is shown in Figure 7.

Knowing that the FPGA works at speed of 50MHz and the line frequency is 60Hz. Using (1); saw-tooth maximum value C_{max} will equal 416666. In (2), C_{θ} can take any value from 0 to 416666 with increment of 1; which allows firing angle to be adjusted with a step of 432*10⁻⁶ degrees.



Figure 6: Voltage, comparator output, and zero-crossing pulse.



Figure 7: Relation between phase voltage, saw-tooth, firing pulses, and FPGA core clock.

Angle Detection and Pulse Duration Counter Block

To generate the firing pulse, the saw-tooth is compared to a constant value C_{θ} respective to the required firing angle. This constant value can be obtained using (2). The firing pulse should starts when the value of sawtooth equals to C_{θ} and stays active for duration equals to ΔC_{θ} . There is a register has an initial value of 0 and will output 1 when being enabled by the saw-tooth comparator. The output of the lower side register is the firing pulse applied to triac gate. Once enabled, the output of lower side register will enable the upper side register. The upper side register and the adder in the top-right corner of the logic diagram form together a digital counter. The counter is incremented every positive edge of FPGA clock and keeps counting up once it's enabled by the lower side register output. The counter will count until it reaches a maximum value of ΔC_{θ} , in this moment the counter and the lower side register are reset in the same time which will disable both the output pulse and the counter in the same time. Also, the lower side register and the counter are reset simultaneously once the phase voltage crossing zero value.

PI Controllers-Blocks

Three PI controllers used to regulate the firing angle position depending on the current mode of operation of the motor and the requested motor speed. Equation (3) is the idealized model for the continuous PI algorithm.

$$u(t) = k_p e(t) + k_i \int e(t)dt$$
(3)

where: u(t) : is the output of PI controller at time t

e(t) : is the error signal at time t,

 k_p : is the proportional gain constant,

 k_i : is the integral gain constant,

For small sample times the continuous time PI equation can be turned into a difference equation by discretization. The integral term is approximated using trapezoidal integration which requires storage of all past sample errors. The intermediate equation can be transformed into a recursive equation where only the previous output, current error, and the last error must be stored. The final discrete version of the PI equation is shown in the following;

 $u(n) = u(n-1) + k_1 e(n) + k_2 e(n-1)$ (4)

The same structure used for the three PI controllers but each controller has different set of constants (k_1 and k_2) based on its k_p and k_i values. Each PI controller was first designed in time domain to set the correct values of k_p and k_i constants. PSIM simulation software used to tune each PI independently. The digital structure of PI controller requires only two multiplications and three additions which is a simple and straight forward algorithm to be implemented using FPGA cells. FPGA already has embedded multipliers blocks (18x18) to be used in the multiplication processes while the addition process is efficiently mapped to FPGA logic cells by synthesis tool. Pipelining registers added after each level of PI structure to post performance and avoid any timing issues due to unbalanced delay in the digital PI structure. The sequencer or the control state machine is a simple control logic used to enable the last stage register (used for u(n)) three clock cycles after receiving new error value e(n). The three PI controllers receive the error signal results from comparing motor sensed speed output from speed sensor and ADC subsystem and the reference speed. The reference speed may be changed online using simple push-buttons.

Limits Decoder Block

The limits decoder block is that part of system which responsible to decide which PI controller to be used based on the current mode of motor operation. The limits decoder block uses two analog comparators for each phase current and simple decode logic inside FPGA. The motor mode of operation is decoded every one complete cycle of phase voltage as a minimum of one complete cycle is needed to determine motor mode of operation based on concept discussed in introduction. Figure 8 shows the analog/digital circuits used in limits decoder block.

Each phase current has a one of two possible states in a complete phase voltage cycle. It can have a zero value or a non-zero value. One analog comparator will generate a positive pulse only if the phase current has a positive value and the other will generate a positive pulse only if the phase current has a negative value. Both comparators will generate a zero output if the phase current has a zero value. Applying the output of two comparators to a logical OR function will result in a logic 1 only if the phase current has a non-zero value.

A stage of decode logic based on AND/NAND logic functions and single bit registers used to decode the three possible states of phase currents. The decoded current states applied to 3-inputs Look Up Table (LUT) which generates the proper control MUX selection signal (selects between 3 different PI controllers). The control MUX selection signal is updated every one complete cycle of phase voltage.

F. Firing Angle Control-block

PI controllers adjust the firing angle so the motor maintains its speed at different loads and mode of operations. The output of selected PI controller must be scaled and clipped to fall in the allowable firing angle range. The firing angle control block receives the selected PI controller output and scales it. The scaled output is compared to maximum and minimum allowable firing angle values and passed only if it falls within the allowable range. If the firing angle value exceeds the maximum allowable value; the value is blocked and only the maximum allowable value is passed. If the firing angle is lower than the minimum allowable value; the value is blocked and only the minimum allowable value is passed. The firing angle is updated every half cycle of phase voltage.

DESIGN IMPLEMENTATION

Control logic was implemented on a Xilinx Spartan-3E embedded development kit. The kit integrates a Spartan-3E FPGA device with over 33,000 of configurable logic cells (UG257, MicroBlaze). The device is intended for cost sensitive embedded applications; however the supported resources and speed allow efficient implementations of digital control systems with performance much better than soft implementations using microcontrollers and DSP processors.

PicoBlaze is an embedded soft processor designed by Xilinx for FPGA applications (UG129, PicoBlaze). One instance of a PicoBlaze processor is used to interface control logic to on-board analog to digital converter circuitry. The PicoBlaze runs an assembly code written independently and compiled using the assembler which produce a VHDL code to integrate into the design.

The whole design is written in VHDL using Xilinx ISE 9.2 design suite. Each part of the control system is written as a separate module to simplify simulation and debugging process. All modules integrated together, synthesized, implemented, and downloaded to the board for system evaluation.

ISE synthesis and implementation tools report a maximum clock speed of 75MHz and utilization of less than 35% of available device resources. This means that the design could be implemented on a smaller FPGA device to reduce design cost and power consumption.

EXPERIMENTAL RESULTS

The three-phase induction motor used in the study is a 380V, 3.81 A, 1.0 kW, 60 Hz and 4 poles, slip ring with the same ratings as used in simulation. The power circuit has been implemented on one board in the lab especially for this paper is shown in Figure 9. This board can be used with any different control devices as microcontroller or PIC controller.

The board circuit consists of the following:

- 1- Three power triacs (Part # BT139) has a 600V Repetitive peak off-state voltage and 16 A on-state current.
- 2- Three opto-coplers (Part # TLP3022).
- 3- 680 current limiting resistors between the triacs and optocopler.
- 4- One dc power supplies +5/-5V to feed the comparators required for zero crossing.
- Three operational amplifiers for zero crossing comparators.
- 6- Three step down transformers to feed the phase voltages to the three comparators.
- 7- Snubber circuit to protect the power Triacs.
- 8- Three current sensors (Part# ACS754KCB) with ±150A sensible current range and 13.3mV/A sensitivity.

The experimental waveforms of three-phase voltages in modes 0/2/3, 2/3, and 0/2 are shown in Figures :10 and 11 respectively. The experimental waveforms of three-phase currents in modes 0/2/3 and 2/3 are shown in Figures 12 and 13 respectively. It is clear from these figures that the line current in the mode 2/3 has the lowest harmonic contents and has the near sinusoidal shape.



Figure 8 Decoding mode and selecting the proper PI controller.



Figure 9 The photo of the complete system.



Figure :10 Three phase voltages in mode 0/2/3.



Figure :11 Three phase voltages in mode 0/2/3.



Figure 12 Three phase currents in mode 0/2/3.





CONCLUSIONS

Three-phase ac voltage controller has been used to start and control the speed of induction motor by controlling the stator voltage. Computer simulation using PSIM and SIMULINK software has been carried out to configure the performance of the motor in each mode. From simulation results there are three modes of operations depending on the shape of supply currents. These modes namely 0/2, 0/2/3, and 2/3. The variation of speed with firing angle is different in each mode. A digital control system has been implemented using FPGA. The control system detects the mode of operation to provide the switches with the correct firing angle. All components of the control system have been designed on FPGA chip. The operating limits have been determined from the simulation results using PSIM and SIMULINK computer program. The experimental results prove the simulation results and show the superiority of the digital control system.

VII ABBREVIATIONS

FPGA	Field Programmable Gate Array		
THD	Total Harmonic Distortion		
PI	Proportional Integrator		
ADC	Analog to Digital Converter		
MUX	Multiplexer		
FF	Flip Flop		
LUT	Look Up Table		
VHDL	Very High Speed Integrated Circuits Hardware		
	Description Language.		

LIST OF SYMBOLS

F	Frequency of phase voltage
t _c	Period of FPGA core clock signal
f_c	Frequency of FPGA core clock signal
C _{max}	Maximum value of digital saw-tooth
C_i	Instantaneous value of digital saw-tooth
θ_i	Instantaneous value of phase voltage angle
C_{θ}	Saw-tooth value respective to a phase voltage angle of θ
θ_p	Duration of firing pulse measured in degrees
ΔC_{θ}	Duration of firing pulse as the difference between saw-tooth value respective to firing angle and saw- tooth value respective to the angle where the firing pulse deactivated.
e(t)	Error signal input to analog PI controller
u(t)	Output of analog PI controller
k _p	Proportional constant of analog PI controller
k _i	Integral constant of analog PI controller
e(n)	Error signal input to digital PI controller at sample n
e(n-1)	Error signal input to digital PI controller at sample <i>n</i> -1
u(n)	Output of digital PI controller at sample n
u(n-1)	Output of digital PI controller at sample <i>n</i> -1
k_1	First constant of digital PI controller
u(n)	Second constant of digital PI controller

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Multi-Resolution and Granular Modelling

MODE-INDEPENDENT STATE FEEDBACK DESIGN FOR DISCRETE SWITCHED LINEAR SYSTEMS

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KEYWORDS

Switched systems, Mode-independent state feedback, Switched Lyapunov function, LMI

ABSTRACT

This paper addresses the stabilization problem of discrete switched linear systems. When the mode is available, a mode-dependent state feedback controller is developed. The main contribution of this note is to provide a less conservative approach to design the mode-independent state feedback controller where the switching mode is not accessible. Both design procedures are expressed in terms of linear matrix inequalities (LMIs). In fact, the new approach provides a family of LMI parameterized by a scalar variable which makes it useful for designing a mode-independent controller and offering an additional degree of freedom. Numerical evaluation is provided to show the effectiveness of the proposed conditions.

INTRODUCTION

Switched linear systems is a class of systems that has been an attractive subject of research during the last decades since it is an appropriate class of systems to model the behavior of practical systems. They are dynamical systems simultaneously containing mixtures of logic and continuous dynamics (D.Liberzon et al., 1999; A.S.Morse,1996). A switched system is represented by a set of continuous-time or discrete-time subsystems and a rule that orchestrates the switching among them. The motivation for studying switched systems is from the fact that many practical systems are required to describe their hybrid behaviour which may depend on various environmental factors and also because the modelling of many complex systems is only possible through combination of the classical continuous laws of control with a logical discrete technique(M.Zefrani et al., 1998). Another source of motivation for studying switched systems comes from the rapidly developing area of switching control. Control techniques based on switching between different controllers have been applied extensively in recent years, particularly in the adaptive context, where they have been shown to achieve stability and improve transient response. The importance of such control methods also stems in part from the existence of systems that cannot by asymptotically stabilized by a single continuous feedback control law. Switched systems have numerous applications in control of mechanical systems, the automotive industry, aircraft and air traffic control, switching power converters, and many other fields which include the modelling of communication networks, networked control systems, the modelling of bio-chemical reactions, the control of nonlinear systems that cannot be stabilized by continuous control laws, the control of systems with large uncertainty using logic-based supervisors, etc. The classical example is the case of continuous time processes that are supervised using logical decision making algorithms. In recent years, particular efforts of researches have received an increasing interest and a growing attention in the study of the stability analysis and control design for switched systems (D.Liberzon et al., 1999; Hui Ye et al., 1995). We address the stability issues and control synthesis for discrete switched systems under arbitrary switching sequences.

In fact, much efforts has been devoted to establishing analysis tools such as multiple Lyapunov functions(MLF), piecewise Lyapunov function (PLF) and switched Lyapunov function (SLF)(M.S.Branicky,1998) (D.Koutsoukos et al., 2002; R.DeCarlo et al., 2000). The approach used in this note is based in the existence of a particular quadratic Lyapunov function making full use of switching nature of the switched system, specially it has the same switching signals as the switched system. It is called SLF (Switched Lyapunov Function) which is a switching-sequence dependent Lyapunov function. It is proved in this note that with the use of switched lyapunov function less conservative results can be obtained (J.Daafouz et al., 2001; J.Daafouz et al., 2002). So, the results proposed in this work can be considered as a tradeoff between higly conservative results (those using a single quadratic Lyapunov function) and less conservative results. The stabilization problem of this class of systems has attracted a lot of researchers and interesting results were reported. For the synthesis of control switched systems with mode-independent controller limited research has been done. In fact, the results obtained using the classical quadratic approach (with a single quadratic Lyapunov function) leads to a highly con-

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) servative results. Moreover, most of the existing results on the stabilization of the switched system require the critical assumption on the accesssibility of the switching mode.Practically, this assumption may sometimes be hard to satisfy and therefore, the developed results are restrictive. One alternative way is to overcome the availability of the switching mode which consists of estimating the mode and then use the existing results. On the other hand, the mode independent controller is very attractive due to its simple structure. To design such controllers, two approaches can be adopted. The first one employs a constant Lyapunov function, which makes the design problem formulated as a linear matrix inequality (LMI) problem. The second one uses mode-dependent Lyapunov function, which usually leads to less conservative results.

This note is organised as follows. In section II, we introduce the problem formulation and we give some preliminaries. Section III, stability analysis of switched systems by mean of a switched quadratic Lyapunov function is stated. Section IV covers the design of stabilizing state feedback under the assumption of the complete access to the state vector and the switching mode. On the other hand, practically, the complete access for the switching mode may not be possible for some applications and a design of mode-independent state feedback controller is of great interest in this case. A numerical evaluation is provided in section VI.

NOTATION

The notations used throughout the paper are standard. The relation A > B (A > B) means the matrix A - B is positive (negative) definite. The matrix I denotes identity matrix of appropriate dimension. • is used for the blocks induced by symmetry. N is the amount of subsystems. Conv{} stands for convex combination.

PROBLEM FORMULATION AND PRELIMINAR-IES

Consider linear switched system in discrete domain described by the following state equation:

$$\begin{cases} x(k+1) = A_{\alpha}x(k) + B_{\alpha}u(k) \\ y(k) = C_{\alpha}x(k) \end{cases}$$
(1)

Where

 $x(k) \in \mathbb{R}^n$ is the state vector of the system, $u(k) \in \mathbb{R}^m$ is the control input, $y(k) \in \mathbb{R}^p$ is the measured output, $\alpha_i(k)$ is the switching signal.

$$\alpha_i(k): Z^+ \to \{0,1\}, \sum_{i=1}^N \alpha_i(k) = 1, k \in Z^+ = \{0,1,...\}$$

It specifies which subsystem will be activated at a certain discrete time.

Remark: The model defined by (1) naturally imposes a discontinuity on A_{α} since this matrix must jump instantaneously from A_1 to A_1 for some $i \neq j$ once switching

occurs. In other words, A_{α} is constrained to jump among N vertices of the vector polytope $conv\{A_1, ..., A_N\}$

Furthermore, for a particular switching laws the switched system can be viewed as a special case of a time-varying linear system and therefore the usual definitions of stability can be used, see for example (R.DeCarlo et al.,2000).

We present now two useful lemmas used in proof.

Lemma 1. (**Projection Lemma**) Given a symmetric matrix $\Psi \in IR^{m \times m}$ and two matrices P, Q of column dimension m there exists X such that the following LMI holds: $\psi + P^T X^T Q + Q^T X P < 0$ if and only if the projection inequalities with respect to X are satisfied $N_P^T \psi N < 0, N_Q \psi N_Q^T < 0$ where N_p and N_Q denote arbitrary bases of the nullspaces of P and Q respectively.

Proof. See (S.Boyd et al., 1994)

Lemma 2. Let Φ a symmetric matrix and N,J matrices of appropriate dimensions. The following statements are equivalent:

(i) $\Phi < 0$ and $\Phi + NJ^T + JN^T < 0$

 $\begin{bmatrix} (ii) & There & exists & a & matrix & G & such & that: \\ \Phi & J + NG \\ J^T + G^T N^T & -G - G^T \end{bmatrix} < 0$

Proof.The proof is obtained remarking that: $\begin{bmatrix} \Phi & J + NG \\ J^T + G^T N^T & -G - G^T \end{bmatrix} = \begin{bmatrix} \Phi & J \\ J^T & 0 \end{bmatrix} + \begin{bmatrix} N \\ -I \end{bmatrix} G \begin{bmatrix} 0 & I \end{bmatrix} + \begin{bmatrix} 0 \\ I \end{bmatrix} G^T \begin{bmatrix} N^T & -I \end{bmatrix}$ and applying lemma 1.

PROBLEM

Here, we are interested in stability analysis and control synthesis problems for this class of switched system. By stability analysis, we mean stability analysis of the origin for the autonomous switched system. A method for control synthesis is provided by using switched Lyapunov function in order to find a state feedback controller. Both design procedures of mode-dependent and modeindependent state feedback are considered. Because, the problem of estimation of the switching times makes the operation of detection mode difficult. Switched systems are systems subject to abrupt changes in their structure and parameters. They are well suited to represent dy-

(2) namic systems subject to switches between alternative configurations. This kind of systems represents some limitation in the identification of the operating mode. So, finding a fixed controller is in this case interesting. A method for control synthesis is provided by using switched Lyapunov function in order to find a modeindependent state feedback control.

$$u(k) = Kx(k) \tag{3}$$

ensuring stability of the closed loop switched system

$$x(k+1) = (A_{\alpha} + B_{\alpha}K)x(k)$$
(4)

STABILITY ANALYSIS

In this section, we address the problem of stability analysis of the origin of an autonomous switched system given by:

$$x(k+1) = A_{\alpha}x(k) \tag{5}$$

Define the indicator function:

 $\alpha(k) = [\alpha_1(k), ..., \alpha_N(k)]^T.$

Then, the switched system can also be written as:

$$x(k+1) = \sum_{i=1}^{N} \alpha_i(k) A_i x(k)$$
(6)

When:

 $\alpha_i(k) = \begin{cases} 1 \text{ when the ith mode Ai is activated} \\ 0 \text{ otherwise} \end{cases}$

To check stability of the switched system, we use this switched Lyapunov function defined as:

$$V(k, x(k)) = x(k)^T P(\alpha(k))x(k)$$
(7)

$$V(k, x(k)) = x(k)^T \left(\sum_{i=1}^N \alpha_i(k) P_i\right) x(k)$$
(8)

With $P_1, ..., P_N$ symmetric positive definite matrices. If such a positive definite Lyapunov function exists and $\Delta V(k, x_k) = V(k + 1, x_{k+1}) - V(k, x_k)$ is negative definite along the solution of (6) then the origin of the switched system given by (5) is globally asymptotically stable as shown by the following general theorem.

Theorem 3. The equilibrium 0 of (J.Daafouz et al., 2002)

$$x(k+1) = f_k(x(k)) \tag{9}$$

Is globally uniformly asymptotically stable, if there exists a function $V : \mathbb{Z}^+ \times \mathbb{R}^n \to \mathbb{R}$ such that:

• V is a positive definite function, decrescent and radially unbounded

• $\Delta V(k, x_k) = V(k+1, x_{k+1}) - V(k, x_k)$ is negative definite along the solution (6)

The Lyapunov function (8) is a positive definite function, decrescent and radially unbounded since

$$V(k,0) = 0 \ \forall \ k \ge 0 \tag{10}$$

And

$$egin{array}{rcl} eta_1 \left\|x_k
ight\|^2 &\leq V(k,x_k) &= x_k^T(\sum\limits_{i=1}^Nlpha_i(k)P_i)x_k &\leq \ eta_2 \left\|x_k
ight\|^2 \end{array}$$

For all $x(k) \in \mathbb{R}^n$ and $k \geq 0$ with $\beta_1 = \min_{i \in I} \lambda_{\min}(P_i)$ and $\beta_2 = \max_{i \in I} \lambda_{\max}(P_i)$ positive scalars.

Proof. See (Vidyasagar, 1993)

MAIN RESULT

In the following theorem, we give four equivalent necessary and sufficient conditions for the existence of the Lyapunov of the form (8) whose difference is negative definite, proving asymptotic stability of (6).

Theorem 4. The following statements are equivalents

(i) There exists a Lyapunov function of the form (8) whose difference is negative definite, proving asymptotic stability of (6)

(ii) There exist N symmetric matrices $P_1, ..., P_N$ satisfying

$$\begin{bmatrix} -P_i & A_i^T P_j \\ P_j A_i & -P_j \end{bmatrix} < 0 \ \forall \ (i,j) \in I \times I$$
 (11)

The Lyapunov function is then given by:

$$V(k, x(k)) = x(k)^T \left(\sum_{i=1}^N \alpha_i(k) P_i\right) x(k)$$

Ie: $\Delta V(k, x_k) = 0 \forall k \ge 0 \text{ and } \Delta V(k, x_k) \le \gamma(\|x_k\|) \forall k \ge 0 \forall x_k \in \mathbb{R}^n \text{ where } \gamma \text{ is of class } K.$

[A function $\gamma : [0, \infty) \to [0, \infty)$ is of class K if it is continuous, strictly increasing, zero at zero and unbounded $(\gamma(s) \to \infty \text{ as } s \to \infty)$]

(iii) There exist N symmetric matrices $S_1, ..., S_N$ and N matrices $G_1, ..., G_N$ satisfying

$$\begin{bmatrix} -G_i - G_i^T + S_i & G_i^T A_i^T \\ A_i G_i & -S_j \end{bmatrix} < 0 \ \forall \ (i,j) \in I \times I \ (12)$$

The Lyapunov function is then given by:

 $V(k, x(k)) = x(k)^T \left(\sum_{i=1}^N \xi_i(k) S_i^{-1}\right) x(k)$ (iv) There exist N symmetric matrices $S_1, ..., S_N$ and

N matrices $G_1, ..., G_N$ satisfying

$$\begin{bmatrix} \alpha_i^2 S_i - S_j & A_i G_i + \alpha_i G_i - \alpha_i S_i \\ \bullet & S_i - G_i - G_i^T \end{bmatrix} < 0 \ \forall \ (i, j) \in I \times I \ (13)$$

 α_i being arbitrary and $\alpha_i \in]-1,1[$. The Lyapunov function is then given by:

$$V(k, x(k)) = x(k)^T \left(\sum_{i=1}^N \alpha_i(k) S_i^{-1}\right) x(k)$$

Proof.

• To prove $(i) \Leftrightarrow (ii) \Leftrightarrow (iii)$ see (J.Daafouz et al.,2002)

• To prove $(ii) \Leftrightarrow (iv)$ assume that:

$$\begin{bmatrix} -S_i & S_i A_i^T \\ \bullet & -S_j \end{bmatrix} < 0$$
Which can be written as:
$$\begin{bmatrix} -S_i & S_i A_i^T \\ \bullet & -S_j \end{bmatrix} =$$

$$\begin{bmatrix} -S_i & -\alpha_i S_i \\ -\alpha_i S_i & -S_j \end{bmatrix} + \begin{bmatrix} S_i \\ 0 \end{bmatrix} \begin{bmatrix} 0 & A_i^T + \alpha_i I \end{bmatrix}$$

$$+ \begin{bmatrix} 0 \\ A_i + \alpha_i I \end{bmatrix} \begin{bmatrix} S_i & 0 \end{bmatrix} < 0$$

with $\Phi < 0$, for all $\alpha_i \setminus -1 < \alpha_i < 1$.

By applying lemma2, this equivalent to the existence of matrices G_i such that:

$$\begin{bmatrix} -S_i & -\alpha_i S_i & S_i \\ -\alpha_i S_i & -S_j & A_i^T G_i + \alpha_i G_i \\ S_i & G_i^T A_i^T + \alpha_i G_i^T & -G_i - G_i^T \end{bmatrix} < 0$$
Which is equivalent by the schur complement to:
$$\begin{bmatrix} -S_j & A_i G_i + \alpha_i G_i \\ \bullet & -G_i - G_i^T \end{bmatrix}$$

$$+ \begin{bmatrix} -\alpha_i S_i \\ S_i \end{bmatrix} S_i^{-1} \begin{bmatrix} -\alpha_i S_i & S_i \end{bmatrix} < 0$$

$$\begin{bmatrix} \alpha_i^2 S_i - S_j & A_i G_i + \alpha_i G_i - \alpha_i S_i \\ \bullet & S_i - G_i - G_i^T \end{bmatrix} < 0$$
Becomerical

Remarks:

• In particular, for $\alpha_i = 0$, we found the results developed in (J.Daafouz et al.,2002)

• for $\alpha_i \in [-1, 1[$, we obtain a family of LMIs conditions parametrized by α_i

MODE-DEPENDENT STATE FEEDBACK DESIGN

Consider the synthesis of a switched static mode-dependent state feedback.

$$u(k) = K_{\alpha} x(k) \tag{14}$$

guaranting stability of the closed-loop switched system (6). This problem reduces to find P_i and K_i ($\forall i \in I$), such that:

$$\begin{bmatrix} -P_i & (A_i + B_i K_i)^T P_j \\ P_j (A_i + B_i K_i) & -P_j \end{bmatrix} < 0 \quad (15)$$

 $\forall (i,j) \in I \times I$ Or equivalently to find S_i , G_i and K_i Such that

$$\begin{bmatrix} -G_i - G_i^T + S_i & G_i^T \left(A_i + B_i K_i\right)^T \\ \left(A_i + B_i K_i\right) G_i & -S_j \end{bmatrix} < 0 \quad (16)$$

 $\forall (i,j) \in I \times I$

Theorem 5. If there exist symmetric matrices S_i , matrices G_i and R_i ($\forall i \in I$) such that $\forall (i, j) \in I \times I$

$$\begin{bmatrix} S_i - G_i - G_i^T & (A_i G_i + B_i R_i)^T \\ A_i G_i + B_i R_i & -S_j \end{bmatrix} < 0$$
(17)

Then the mode-dependent state feedback given by (14) with

$$K_i = R_i G_i^{-1} \ \forall \ \mathbf{i} \in \mathbf{I} \tag{18}$$

asymptotically stabilizes (1).

• The next section shows that the contribution of Theorem 4 is to propose a condition which is less conservative for the problem of a Mode-Independent state feedback.

MODE-INDEPENDENT STATE FEEDBACK CONTROLLER

The results of the previous section assume the complete access of the switching mode. Practically, this may not be possible for some application and a design of mode-independent state feedback controller is of great interest in this case. We now seek a stabilizing modeindependent control law given by:

$$u(k) = Kx(k) \tag{19}$$

where $K \in \mathbb{R}^{n_u \times n}$ is a constant matrix. This approach may be restrictive compared to mode-dependent state feedback controller but has less conservative to what has been reported in the literatures(those using a single quadratic Lyapunov function).

The following theorems provide conditions for finding a mode-independent state feedback controller.

Theorem 6. If there exist symmetric matrix P, a matrix R Such that

$$\begin{bmatrix} -P & (A_iP + B_iR)^T \\ \bullet & -P \end{bmatrix} < 0 \ \forall \ i \in I$$
 (20)

Then the mode independent state feedback controller is given by:

$$K = RP^{-1} \forall i \in I \tag{21}$$

Theorem 7. If there exist symmetric matrices S_i , a matrix G, a matrix R and arbitrary prescribed numbers $\alpha_i \in [-1, 1[$ such that: $\forall (i, j) \in I \times I$

$$\begin{bmatrix} \alpha_i^2 S_i - S_j & A_i G + B_i R + \alpha_i G - \alpha_i S_i \\ \bullet & S_i - G - G^T \end{bmatrix} < 0$$
(22)

Then the mode independent state feedback controller is given by:

$$K = RG^{-1} \;\forall \; \mathbf{i} \in \mathbf{I} \tag{23}$$

Theorem 8. Letting $R_i = KG_i \forall i \in I$ and $G_i = \alpha_i G \forall i \in I$, If there exist symmetric matrices S_i , matrices G_i , matrices R_i and arbitrary prescribed numbers $\alpha_i \in]-1, 1[$ such that $\forall (i, j) \in I \times I$

$$\begin{bmatrix} \alpha_i^2 S_i - S_j & \alpha_i A_i G + \alpha_i B_i K G + \alpha_i^2 G - \alpha_i S_i \\ \bullet & S_i - \alpha_i G - \alpha_i G^T \end{bmatrix} < 0$$
(24)

Then the mode independent state feedback controller is given by:

$$K = RG^{-1} \forall i \in I$$
 (25)

NUMERICAL EVALUATION

In this section, a numerical evaluation is proposed. The problem considered here is the design of a static mode-independent state feedback controller stabilizing the switched system. The result obtained using the theorem (8) is compared to the three methods given by the theorems (5), (6), (7) and summarize in the table 1. The switched system is characterized by: the number of modes (N), the system order (n), number of inputs (m) and the number of outputs (p). For fixed values of (N, n, m, p), we generate randomly 100 switched systems of the form (1). So the purpose is to design by using the four methods a feedback controller in the form (2) such that the closed -loop system is asymptotically stable.

• Method 1: uses constant Lyapunov function $(CLF)V(x_k) = x_k^T P x_k.$

and applying the conditions given in Theorem 6.

• Method 2: uses the conditions given in Theorem 7.

• Method 3: uses the conditions given in Theorem 8.

• Method 4: uses the conditions given in Theorem 5. By using the matlab LMI Control Toolbox to check the feasibility of the LMI conditions, we introduce a counter (Success Method1, Success Method2, Success Method3 and Success method4) which is increased if the corresponding method succeeds in providing an state feedback stabilizing control.

SUMMARY AND CONCLUSIONS

In this paper, the problem of stability and synthesis of discrete switched linear systems using switched Lyapunov function (SLF) is investigated. Tow types of controllers were designed using the LMI setting. The first one assumes the complete access to the switching modes which gives mode-dependent controller. The second one relaxes this assumption and a mode-independent gain is obtained which may be restrictive compared to modedependent state feedback controller but has less conservatism to what as been reported in the literatures. The derived conditions, are expressed as a family of linear matrix inequalities (LMIs)parameterized by the scalar variables α_i . These conditions reduce significantly the conservatism and show the advantage of using the scalar variables in the case of mode-indepent state feedback. Numerical evaluations are given to demonstrate the applicability and the conservatism reduction of the proposed conditions and a comparison with recent conditions proposed in the literature has been described.

Table I: Nu	merical Eval	uation	
Switched System	Success	N=2	N=3
n=3	Method 1	97	88
m=1	Method 2	100	96
p=1	Method 3	100	98
	Method 4	100	100
n=4	Method 1	91	77
m=1	Method 2	100	82
p=1	Method 3	100	86
	Method 4	100	100
n=5	Method 1	90	49
m=1	Method 2	98	64
p=1	Method 3	98	64
	Method 4	100	100
n=4	Method 1	100	97
m=2	Method 2	100	99
p=1	Method 3	100	99
	Method 4	100	100
n=5	Method 1	100	93
m=2	Method 2	100	96
p=1	Method 3	100	96
	Method 4	100	100
n=4	Method 1	94	77
m=1	Method 2	100	84
p=2	Method 3	100	84
	Method 4	100	100
n=5	Method 1	88	46
m=1	Method 2	97	56
p=2	Method 3	97	62
	Method 4	100	100
n=7	Method 1	96	36
m=2	Method 2	100	83
p=1	Method 3	100	89
	Method 4	100	100

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MULTI-RESOLUTION MODELLING OF TOPIC RELATIONSHIPS IN SEMANTIC SPACE

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KEYWORDS

Document modelling, Probabilistic topic models, Latent semantic allocation, Topic hierarchy

ABSTRACT

Recent techniques for document modelling provide means for transforming document representation in high dimensional word space to low dimensional semantic space. The representation with coarse resolution is often regarded as being able to capture intrinsic semantic structure of the original documents. Probabilistic topic models for document modelling attempt to search for richer representations of the structure of linguistic stimuli and as such support the process of human cognition. The topics inferred by the probabilistic topic models (latent topics) are represented as probability distributions over words. Although they are interpretable, the interpretation is not sufficiently straightforward for human understanding. Also, perhaps more importantly, relationships between the topics are difficult, if not impossible to interpret. Instead of directly operating on the latent topics, we extract topics with labels from a document collection and represent them using fictitious documents. Having trained the probabilistic topic models, we propose a method for deriving relationships (more general or more specific) between the extracted topics in the semantic space. To ensure a reasonable accuracy of modeling in a given semantic space we have conducted experiments with various dimensionality of the semantic space to identify optimal parameter settings in this context. Evaluation and comparison show that our method outperforms the existing methods for learning concept or topic relationships using same dataset.

INTRODUCTION

Document modelling has its roots in Information Retrieval (IR) and aims to provide suitable document representation to facilitate efficient processing of information for retrieval systems. One of the classic IR models, the Vector Space Model (Baeza-Yates and Ribeiro-Neto, 1999), represents a document as "bag-of-words" which is a high dimensional word vector of weighted terms that are computed by combining the "terms frequency" and "inverse document frequency" (Baeza-Yates Andrzej Bargiela School of Computer Science University of Nottingham Malaysia Campus Jalan Broga, 43500, Semenyih, Selangor, Malaysia Email: abb@cs.nott.ac.uk

and Ribeiro-Neto, 1999). The retrieval process is realised by computing Cosine similarity between the query and document vectors. Another classic model, Probabilistic model (we focus on the Binary Independence model) (Robertson and Jones, 1976) makes an assumption of "binary independence" between terms in a document, which is represented as a high dimensional binary vector in the word space. The retrieval process with regard to a query is done by estimating weights of each term presented in the query. The two classic and some extended IR models emphasise the co-occurrence of terms between queries and documents, for example, as the Vector Space model, "term frequency" is also included in the popular Okapi BM25 (Robertson et al., 1998) term weighting scheme.

One of the problems associated with the abovementioned two models is that if terms do not co-occur in queries and documents, the retrieval performance deteriorates significantly. This problem is attributed to a great extent to the phenomenon of synonymy and polysemy [Deerwester1990] present in natural languages. There have been some works towards deriving low dimensionality representation of the documents in the socalled semantic space, such as Latent Semantic Analysis (LSA) (Deerwester et al., 1990), probabilistic variants of Latent Semantic Analysis (pLSA) (Hofmann, 1999), and Latent Dirichlet Alllocation (LDA) (Blei et al., 2003; Steyvers and Griffiths, 2005; Griffiths and Steyvers, 2004; Steyvers et al., 2006). The intuition is that similarity between documents in the low dimensional semantic space could be higher than the one in the high dimensional word space, even if terms do not cooccur in queries and documents. Among these models, probabilistic topic models (Blei et al., 2003; Steyvers and Griffiths, 2005; Steyvers et al., 2006) aims to search for richer representations of the structure of linguistic stimuli and support the process of human cognition. The technique enables construction of a lower dimensional representation of a document while preserving its semantic structure. Furthermore, the learned topics can be interpreted as probability distribution of words, which can be understood by humans. However, the task of interpretation is not trivial. One needs to scan through the words noting corresponding probability values in learned topics and apply this insight in order to understand the meaning of a topic (i.e., associating a label to a topic). In this

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) context, the relationships between these implicit topics are not clear (i.e., more general or more specific) and the issue has not been discussed in the literature.

In our proposed method, instead of directly operating on the latent topics, we extract topics from a document collection and make use of explicit labels that are intuitive for human understanding. The extracted topics are represented using fictitious documents, compiled as words from the vicinity of the occurrences of the topic labels, or as documents, which are annotated by these labels. These documents are fed to a set of learned probabilistic topic models to derive new representations in the low dimensional semantic space. We then propose a method to derive relationships between topics using a relationship learning algorithm based on "Information Theory Principle for Concept Relationship". Experiments with various dimensionality of the semantic space have been conducted to assess the validity of the proposed method. Empirical evaluation on a representative data set shows that the accuracy of the inferred relationships is up to 85%, which is a notable improvement compared to the results generated using the existing concept relationship learning algorithms (Sanderson and Croft, 1999; Zavitsanos et al., 2007) applied to the same dataset (the comparative study can be found in (Wei et al., 2008)).

The rest of the paper is organised as follows. We first give a brief introduction to the probabilistic topic models, emphasises on the Latent Dirichlet Allocation (Blei et al., 2003; Steyvers and Griffiths, 2005). Then we elaborate our method for learning relationships between topics, in particular, justification of the method, the "Information Theory Principle for Concept Relationship", document modelling in the semantic space with various resolution, and the relationship learning algorithm. After that, we report experimental results under different parameter settings and the comparison with results generated using other approaches. Finally we conclude the paper and discuss issues related to future research.

PROBABILISTIC TOPIC MODELS

Latent Semantic Analysis (LSA) (Deerwester et al., 1990) is introduced to alleviate some of the problems associated with classic IR techniques, i.e., synonymy and polysemy, by computing document representations in a semantic space. Probabilistic extensions of the LSA such as probabilistic Latent Semantic Analysis (pLSA) (Hofmann, 1999) and Latent Dirichlet Allocation (LDA) (Blei et al., 2003; Griffiths and Steyvers, 2004; Steyvers and Griffiths, 2005) have been developed to improve the interpretation of the results generated by the LSA. By contrast to the LSA, which explores the latent semantic space using Singular Value Decomposition, probabilistic models represent semantic properties of words and documents using latent topics interpreted as word-topic and topic-document distributions. These models have shown to be effective dimension reduction techniques (Hofmann, 1999; Blei et al., 2003; Steyvers and Griffiths, 2005).

Latent Dirichlet Allocation

Latent Dirichlet Allocation (LDA) (Blei et al., 2003) is a modelling approach based on probabilistic inference and generalises easily to new documents. It does not suffer from the two problems associated with the probabilistic Latent Semantic Analysis (pLSA), i.e., overfitting (Blei et al., 2003), and the difficulty of generalising to new documents (Steyvers and Griffiths, 2005).

Generative Process

LDA is a generative model: each word w_i in a document is generated by sampling a topic from the topic distribution, and then sampling a word from topic-word distribution. The generative process can be represented using Equation (1) (The notations we use for LDA model follow those used in [Griffiths2004,Steyvers2005]).

$$P(w_i) = \sum_{j=1}^{T} P(w_i | z_i = j) P(z_i = j)$$
(1)

where $P(z_i = j)$ is the probability that *j*th topic is sampled for the *i*th word token, and $P(w_i|z_i = j)$ is the probability of sampling w_i under topic *j*. Let $\phi^{(j)} = P(w|z = j)$ refer to multinomial distribution over words for the topic *j*, and $\theta^{(d)} = P(z)$ refer to multinomial distribution over topics in the document *d*. The ϕ and θ are model parameters that need to be estimated.

Parameter Estimation

There are various algorithms available for estimating parameters in LDA, for example, Blei et al (Blei et al., 2003) introduced the variational inference with Expectation-Maximisation algorithm (Bilmes, 1997). In this paper, we adopt the Gibbs sampling algorithm to estimate parameters in LDA as proposed in (Steyvers and Griffiths, 2005; Griffiths and Steyvers, 2004). The idea is that instead of estimating the topic-word p(w|z) and document-topic p(z|d) distributions directly, one can estimate the posterior probability distribution over latent variable z given the observed data conditioned on topic assignment for all the other word tokens using Equation (2) (see (Steyvers and Griffiths, 2005; Griffiths and Steyvers, 2004)).

$$P(z_{i} = j | \boldsymbol{z}_{-i}, \boldsymbol{w}) \propto \frac{n_{-i,j}^{(w_{i})} + \beta}{n_{-i,j}^{(.)} + W\beta} \frac{n_{-i,j}^{(d_{i})} + \alpha}{n_{-i,.}^{(d_{i})} + T\alpha}$$
(2)

The first term on the right side of the Equation (2) represents the probability of word w under topic j, and the second term in represents the probability of topic j in the document d. Intuitively, the assignment of a word to a topic depends not only on how likely the word is associated with a topic, but also on how dominant is the topic in a document (Steyvers and Griffiths, 2005).

The Gibbs sampling algorithm starts with random assignment of word tokens to topics. Each Gibbs sample consists of topic assignments to all of the word tokens in the corpus. Samples before the "burn-in" period are discarded due to poor estimates of the posterior probability. After the "burn-in" period, a number of Gibbs samples are preserved at regular intervals to prevent correlations between samples (Griffiths and Steyvers, 2004; Steyvers and Griffiths, 2005). The word-topic and topic-document distribution can be obtained using Equation (3) and (4).

$$\hat{\phi}_{j}^{(w)} = \frac{n_{j}^{(w)} + \beta}{n_{i}^{(.)} + W\beta}$$
(3)

$$\hat{\theta}_{j}^{(d)} = \frac{n_{j}^{(d)} + \alpha}{n^{(d)} + T\alpha}$$
(4)

where *n* is count matrix, $n_j^{(w)}$ is the number of word token *w* assigned to topic *j*, $n_j^{(d)}$ is the total number of word tokens assigned to *j* in the corpus, $n_j^{(d)}$ is the number of token assigned to *j* in document *d*, and $n_j^{(d)}$ is the number of tokens in *d*.

Query Folding-in

The query folding-in process involves computing low dimensional representations of either queries or previously unseen documents (Deerwester et al., 1990). The computation can be done using the same algorithm as for parameter estimation during training. We propose here that new documents are folded-in to the learned LDA models using the Gibbs sampling algorithm conditioned on the topic-word probabilities , i.e., keeping the topic-word distributions fixed, and assigning each word to LDA topics in the new document.

LEARNING TOPIC RELATIONSHIP

To avoid the process of manual labeling of documents, we propose to interpret topics through the following three steps.

- extract topics from the dataset;
- represent these topics as documents in the word space;
- fold-in the documents to the trained LDA models to obtain their representations in the low dimensional semantic space.

The first step can be realised by extracting document annotations provided by humans, or by using Information Extraction techniques (Cunningham and Bontcheva, 2005). In general, a topic is a "complex" entity which is normally well-understood by human, and is often in a form of noun-phrase, for example, "Latent Dirichlet Allocation". However, the meaning of the topic is difficult for computers to interpret. The term independence assumption apparently cannot be applied here because it would destroy the intentional structure of the entity and the meaning might be totally different from the intended one.

We represent topics using fictitious documents, which explain those topics in details and formalise a concrete context in which topics are used, for example, words in its vicinity, or documents that are annotated with the topic. The idea coincides with the "distributional hypothesis" (Harris, 1968) which states that similar words tend to appear in similar contexts. These documents are then folded-in to the learned LDA models to derive their low dimensional representations.

Information Theory Principle for Concept Relationship

Before we introduce the "Information Theory Principle for Concept Relationship", The definition for Kullback-Leibler divergence (KL divergence or $D_{KL}(P||Q)$)) (MacKay, 2003) (also known as Relative Entropy) is given to underpin the principle.

Definition 1 The relative entropy or Kullback-Leibler divergence between two probability distributions P and Q over the same discrete space A is defined as: $D_{\text{KL}}(P||Q) = \sum_{i \in A} P(i) \log \frac{P(i)}{Q(i)}$

Following the Gibbs inequality MacKay (2003), KL divergence value is: $D_{KL} > 0$.

Definition 2 A concept C_p is broader than another concept C_q if the following two conditions hold:

- (similarity condition) Similarity measure between C_p and C_q is greater than certain threshold TH_s (or divergence measure is less than certain threshold TH_d), and
- (divergence difference condition) Difference between Kullback-Leibler divergence measures: $D_{KL}(P||Q) - D_{KL}(Q||P) < 0.$

In the above definitions, P and Q are probabilistic distributions of latent topics for concepts Cp and Cq respectively. The similarity measure can be calculated using Cosine similarity (Baeza-Yates and Ribeiro-Neto, 1999) or Jensen-Shannon (JS) divergence measures (MacKay, 2003). The threshold TH can be tuned to achieve satisfactory results.

The semantics of the KL divergence can be explained as the expected number of bits that are wasted by encoding events from the true distribution P with a code based on the not-quite-right distribution Q. It is the average "surprise" due to incoming message being drawn from distribution Q when it is expected to arrive form the true distribution P. Intuitively, given that the first condition holds, if the KL divergence $D_{KL}(P||Q)$ is less than $D_{KL}(Q||P)$, then the concept C_p is said to be more general than concept C_q . An example would help to understand the principle: if a source transmits a concept C (e.g., "Machine Learning"), and a receiver believes that the information received is the true C. However, the actual information he receives is C^* (e.g., "Neural Network"), the KL divergence $KL(C, C^*)$ measures the surprise of the receiver. If C is more general than C^* , we would expect that the first surprise $KL(C, C^*)$ will be smaller than the second one $KL(C^*, C)$.

The Definition 2 in a sense encompasses seemingly opposing tendencies. At one extreme, if two distributions are exactly the same, their respective KL divergences are same. However, calculation based on the LDA representation of the documents shows that the difference between the KL divergences of "close" or similar "distributions" can be extracted as shown in our experiments. Usefulness of the KL divergence also depends on precision of estimation of the involved distributions (which may become problematic for larger event space sizes). The experimental study shows that LDA training based on the use of Gibbs sampling is able to produce accurate estimation results as compared to other latent semantic models. Furthermore, dimensionality of the semantic space determined by the LDA model is far smaller than the original word space, thus the method does not involve computation of KL divergence in large space.

Topic Hierarchy Construction Algorithms

Interpreting relationships between topics individually does not provide an overall view on relations between topics. Based on the principle defined above, we develop a recursive algorithm for learning relationships between topics and constructing topic hierarchies, assuming that a topic can only has one "broader" topic. The basic idea of the algorithm is to search recursively for the most similar topics of the current "root" topic and remove those that do not satisfy the condition on the difference of KL divergence.

The parameters used in the algorithms are shown as follows:

- N The total number of extracted topics.
- M_c The maximum number of sub-nodes for a particular node.
- *TH* The thresholds for similarity and divergence measures.
- TH_n The noise factor, defined with the difference between two KL divergence measures $D_{KL}(P||Q)$ and $D_{KL}(Q||P)$.

The parameters values of TH and TH_n can be tuned to obtain satisfactory recall, precision and F1 values (see Section "Evaluation"). In our experiment we have found that setting TH and TH_n within some narrow ranges results in only slight variation of recall and precision values. M_c is used to assess the effect of maximum number of sub-nodes for a particular node has on accuracy of the results (see (Wei et al., 2008) for detailed discussion on this parameter).

The algorithm starts with specifying the root topic and adding it into the Processing Vector, V. The vector V_{temp} stores the most similar topics of the current "root" node. The selected most similar concepts in V_{temp} are filtered using a two steps procedure:

- Topics whose KL divergence values with the current "root" do not satisfy the divergence difference condition are removed from V_{temp},
- For each concept left in the V_{temp} , a "broader" relation is asserted if the similarity value between the topic and the current "root" is greater than similarity value between the topic and any of the siblings of the current "root".

The algorithm will terminate according to the conditions specified in the while loop. The pseudo-code for the algorithm is given in Algorithm 1.

Algorithm 1 relationLearning(root)
Require: Initialise V, M_s, I, TH, TH_n , and M_c .
Ensure: A terminological ontology with "broader" rela-
tions.
1: Initialise V, M_s, I, TH, TH_n , and M_c ;
2: while $(i < I \text{ and } V \text{ is not empty})$ do
3: Add current root into V ;
4: Select most similar M_c nodes of root from M_s ;
5: Add similar nodes into V_{temp} ;
6: Remove nodes in V_{temp} against Definition 2;
7: for (all nodes n_i in V_{temp}) do
8: if $(Sim(n_i, root) > Sim(n_i, Sibling(root)))$
then
9: Assert broader relations between root
and topic n_i ;
10: end if
11: Move topic n_i from V_{temp} to V ;
12: Increment i by 1;
13: end for
14: Remove current root from V ;
15: end while

In the algorithm, the function Sim(a, b) returns similarity values between nodes a and b. The function Sibling(root) returns a list of siblings of the current "node". Time complexity of the algorithm is $O(m^2 \cdot n^2)$, where $m = M_c$, n = N, and $n \gg M_c$. Since the value of m is much smaller than n, the algorithm is more efficient compared to the one in (Zavitsanos et al., 2007) which has time complexity of $O(n^3)$.

EXPERIMENTS

For the experiment, we have prepared a dataset consists of about 4,600 abstracts of published articles in the area of semantic Web. The dataset was processed by removing stopwords, applying Part-of-Speech (POS) tagging (only nouns, verbs, and adjectives were kept), and stemming, resulting in approximately 6900 unique words in total.

We extracted keyword annotations of the documents. Frequently appearing keywords were used as topics whose relationships were to be learned (77 topics were used in our experiment). A topic was then represented using documents annotated by the topic (i.e., documents were merged; words occurring only once were removed). The resulting document can be viewed as one that describes the particular topic. After probabilistic topic models have been trained, documents representing topics were used as "new documents" and folded into the trained topic models to obtain low dimensionality representations. This study is focused specifically on the exploration of the effect of the variable dimensionality of the semantic space and it builds on the previous publication describing in more detail the methodological issues (Wei et al., 2008).

Training Probabilistic Topic Models

We trained seven LDA models using different number of latent classes, i.e., from 30 to 90, which represents seven different latent spaces with increasing resolution of semantics. This allows to compare the results generated by the relationship learning algorithm in different semantic spaces. For each LDA model, the first 2000 Gibbs samples were dropped due to poor posterior probability estimation. After the "burn-in" period, the subsequent Gibbs samples were preserved to estimate the target probability distributions. The output of the Gibbs algorithm was a set of parameters p(w|z) and p(z|d). These parameters are saved into two matrices for folding-in the documents that represent the extracted topics.

Folding-in New Documents

The topic documents were then folded-in to the seven trained LDA models respectively by using the Gibbs sampling algorithm conditioned on the topic-word probability distributions. Gibbs samples after the "burn-in" period were saved and the output was seven sets of document-topic distributions in the semantic spaces of various dimensionalities. To improve the efficiency of the relationship learning algorithm, two matrices containing pair-wise similarity and KL divergence values between the folded documents are calculated before running the algorithm.

Applying Relationship Learning Algorithm

The topic hierarchy construction procedure is a straightforward process once the topic models were learned and new documents were folded-in. In our experiment, we have used different combinations of parameters to find optimal settings, for example, the number of classes (from 30 to 90, representing various dimensionality of the semantic space), and maximum number of subnodes and the use of similarity measures. (due to the space limitation, effects of these parameters are not discussed in this paper. See (Wei et al., 2008) for more details). We have achieved a satisfying balance between the recall and precision measures by setting the range of similarity threshold $TH \subset [0.5, 0.75]$ for Cosine similarity measure, or $TH \subset [0.25, 0.45]$ for JS divergence measure, and the noise factor $TH_n \subset [0.3, 0.5]$.

A number of topic hierarchies have been constructed using the topic hierarchy learning algorithm. Figure 1 shows a snippet of a hierarchy centering on "Ontology" with "broader" relationships. The hierarchy was learned using Cosine similarity measure and LDA model with 40 classes.



Figure 1: A snippet of the ontology centering on the topic "Ontology"

EVALUATION

The results generated by the experiments were evaluated by domain experts. Only if correctness of a relationship is agreed by all domain experts, the relationship is marked as correct. We use recall, precision and F1(Baeza-Yates and Ribeiro-Neto, 1999) which are common measures in Information Retrieval to assessing performance of text retrieval, denoted as R, P, and F1 respectively, to evaluate the performance of our method The recall is defined as:

$$R = \frac{n_{tc}}{N_{cs}} \tag{5}$$

where n_{tc} is the number of correct learned statements given by the algorithms, N_{cs} is the total number of correct statements. It is assumed that a topic can only have one broader topic, thus the value of N_{cs} is equal to $N_c - 1$, where N_c is the total number of concepts. The precision is defined as:

$$P = \frac{n_{tc}}{N_{ls}} \tag{6}$$

where n_{tc} is the number of correct derived relationships, N_{ls} is the total number of retrieved relationships by the algorithm. Precision measure alone is not sufficient for assessing the performance of the algorithm. Low recall signifies that large portion of relationships are not learned by the algorithms. The F1 measure is defined as the harmonic mean of recall and precision.

$$F1 = \frac{2 * R * P}{R + P} \tag{7}$$

Evaluation Results

For each of the seven trained models, topic hierarchies are constructed with different maximum number of subnodes (i.e., from 5 to 10) using the algorithm. Table 1 shows the results of recall, precision and F1 under different parameters settings. Note that the numbers in the table are averaged over maximum number of sub-nodes.

Table 1: Recall measures of ontology statements based on pLSA and LDA

Settings VS	NoOfClasses	30	40	50	60	70	80	90
Recall	COS	0.712	0.746	0.73	0.766	0.744	0.7	0.61
	JS	0.776	0.704	0.61	0.713	0.656	0.632	0.603
Precision	COS	0.712	0.846	0.732	0.771	0.785	0.737	0.722
	JS	0.8	0.76	0.709	0.837	0.743	0.736	0.768
F1	COS	0.712	0.792	0.731	0.768	0.764	0.718	0.661
	JS	0.788	0.731	0.656	0.77	0.697	0.68	0.675

Averaged recall (recall averaged with different number of classes and algorithm settings) of the experiment over all hierarchies is 69.3%, and the highest recall is 77.6% when "JS+LDA30" (JS divergence and 30 classes for training LDA model) is used. The highest precision with the LDA model was 84.6% when the parameters were set to 40 classes, the maximum number of sub-nodes was set to 8, and Cosine similarity measure were used. The lowest precision was about 70.9%. The best F1 value of LDA is 79.2%. We have conducted another experiment using the probabilistic Latent Semantic Analysis (pLSA) (Wei et al., 2008), the overall results were inferior than the ones generated in this experiment. We attribute the superior performance of the LDA model to its capability of generalising to new documents.

Trade-offs in Different Semantic Space

Finding optimal dimensionality of the semantic space is an issue, which echoes the considerations highlighted by "granular computing" in the general context of information-processing (Bargiela and Pedrycz, 2008, 2002). Choosing a suitable dimensionality has to take specific problems and objectives into consideration. For example, trade-offs between the emphasis on performance measures and the computational complexity have to be considered. In LDA, the computational complexity is proportional to the number of LDA classes used for training.

Evaluation of the results of the experiments with the semantic spaces of various dimensionalities allows us to

develop an insight into the significance of this parameter. This is illustrated in Table 1. One of the most notable observations is that the performance measures in terms of recall, precision, and F1 have no strong correlations with the dimensionality of the LDA model. Results generated using LDA classes more than 60 are especially undesirable. Recall measures with dimensionalities of 30 (77.6%) and 60 (76.6%)) are higher than all the other cases, while precision measures with 40 (84.6%) and 60 (83.7%) classes are higher. The highest (averaged) F1 measure is achieved using 60 LDA classes, but the computational complexity is higher than those with lower dimensionalities. Although the choice of an appropriate dimensionality of a semantic space is determined by specific problems, we can safely conclude that the semantic space with 30, 40, and 60 classes is more appropriate for modelling topic relationships than the other alternatives considered here.

CONCLUSION AND FUTURE WORK

The recent developed probabilistic topic models, i.e., Latent Dirichlet Allocation (LDA), view the task of document modelling as a problem of probabilistic inference in which context is appropriately modulated by statistics of the environment (Steyvers et al., 2006). LDA explores a low dimension semantic space for representing documents with varying resolutions and searches for richer representation of the structures of the original documents. With careful interpretation, the learned topics are intuitively understandable for human and can be matched with the topics appearing in document collections.

Nevertheless, relationships such as "more general" or "more specific" between these topics learned using topic models are difficult to derive. In this paper, we have introduced our approach towards modelling such relationships, which does not directly operating on LDA topics. By extracting topics from a document collection and utilising LDA as effective dimension reduction technique, we are able to model relationships between topics. We have conducted experiments in the semantic space with varying resolutions to identify the optimal parameter settings for achieving satisfactory results. In addition, we have performed a comparative study with some of the existing relationship learning methods. Our method achieved notable improvement in terms of recall and precision measures. Therefore, our main contribution is the method for modelling topics relationships using probabilistic topic models, expanding the applicability of topic models to tasks other than document modelling. Another aspect of our contribution is the proposal of "Infomation Theory for Concept Relationship" which uses Kullback-Leibler divergence as a probabilistic proxy for learning topic relationships.

Although our methodology is intuitively domain independent and has produced encouraging results with a computer science publication dataset, future work will include deploying the proposed method in other domains. For datasets from highly diverse domains, one would expect that the LDA training results in several nearly disjoint sub spaces in the semantic space. Representation of a document from one domain will be dominated by LDA topics for that particular domain. However, experiments are needed to verify the statements and we would like to keep this as our future work.

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NEURAL CLUSTERING OF CORRESPONDENCES FOR VISUAL POSE ESTIMATION

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KEYWORDS

Unsupervised Learning, Clustering, Higher-Order Neural Networks, Correspondences, Pose Estimation.

ABSTRACT

This paper is concerned with the problem of visual pose estimation, which entails, for example, the estimation of object translations. It adopts a correspondence based approach in general, and in particular, looks into a neural network implementation of the approach. The objective of the paper is to demonstrate how the approach can be learnt via the unsupervised clustering of correspondences into clusters representing different poses. Purely local (i.e. Hebbian) mechanisms were adopted in order to ensure not only the practical value of the learning algorithm but also its biological relevance. The results of the experiments here reported show that the learning strategy adopted allows for the successful unsupervised clustering of correspondences, even when the environment puts forth several difficult challenges, such as scarce or correlated features.

INTRODUCTION

Vision presents us with a vast array of computational problems, e.g.: object recognition, motion analysis, stereopsis, colour constancy and pose estimation. The problem of estimating a pose involves, for example, determining the position, orientation and size of a particular object. The main objective of the paper is to demonstrate the feasibility of an unsupervised clustering approach to the problem, which furthermore incorporates several neurobiological constraints, such that the approach can be relevant to both real-world applications and the simulation of biological processes.

A large proportion of pose estimation algorithms within theoretical and applied Computer Science are based on correspondences, which are nothing other than vectors defined by two points that represent two matching local features: one in the source pattern and the other in the target pattern. Correspondence based approaches can be roughly divided into two categories: 1) search based and 2) vote based. Search based correspondence approaches (Fischler and Bolles 1981; Ullman 1996; Breuel 1992; Baird 1985) score highly in terms of generality and

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) robustness. falter somewhat hut in terms of parallelizability. computational simplicity and efficiency. Vote based correspondence approaches, which are based on the Hough Transform (Hough 1962; Ballard 1981; Tian and Shah 1997; Espinosa and Perkowski 1991; Lamdan and Wolfson 1988), are the only approaches reviewed so far that render themselves quite naturally to neural implementations. Because we are interested in a biologically relevant (or neural) unsupervised clustering approach to pose estimation, we have chosen to pursue vote based correspondence approaches.

Seeing that correspondences can be represented by multiplicative nodes and that the transformation space can be represented by an array of summation nodes, the whole approach can be elegantly encapsulated by a special case of a Higher Order Neural Network (HONN), which is closely related to sigma-pi networks. The following specializations distinguish the resulting architectures from general HONNs: 1) two input maps rather than one are used, 2) only second order information is represented and 3) second order information is represented between, rather than within maps (i.e. inter-map rather than intra-map conjunctions). Refer to Figure 1 for a diagram of an artificial neural architecture solving a highly simplified one-dimensional pose estimation problem (i.e. shifts of -1, 0 or +1 pixels).



Figure 1: Pose estimating artificial neural network.

The current paper aims to demonstrate how simple local mechanisms, governed by Hebb-like rules (Hebb 1949), in association with coherent visual stimulation, are sufficient for implementing unsupervised learning of the pose estimating connectivity alluded to in Figure 1 (i.e. the connectivity between correspondence detectors and vote nodes). Note that correspondence detectors, are essentially conjunctions (or multiplicative nodes) between maps, representing whether a particular correspondence between features is being manifested or not, e.g.: if feature F1 at location L1 and feature F1 at location L2 are both active at time t1, then the correspondence between L1 and L2 should be detected at that time.

From the perspective of Granular Computing, the transformation from the input layer to the vote node layer, can be seen to be imposing a specific granulation, resulting from the unsupervised clustering of correspondence detectors at different vote nodes (i.e. poses), and realizing two different resolutions of pose estimation differentiated in terms of accuracy (i.e. correspondence detectors represent poses with limited accuracy whereas vote nodes represent poses with significant levels of accuracy). So far, to the best of our knowledge, the problem of pose estimation has never been solved via the unsupervised clustering of correspondences.

METHODS

Our simulated environment, responsible for providing visual information to the network, consists of two elements: 1) a static image and 2) a dynamic window. The dynamic window is allowed to move around the image. continuously conveying the underlying information to the developing neural network. More specifically, at each iteration, the window contents of both the current and the previous time steps are conveyed to the network. The transformation (or pose) relating the contents of the window at both time steps recovers the motion undergone by the window. Thus motion analysis in this context can be addressed as a pose estimation problem. By controlling the motion of the window, we control the type of pose estimation problem that the developing neural architecture is confronted with. By controlling the nature of the underlying static image we can control environmental factors that may or may not influence the clustering process.

Our learning algorithm consists of the following four main elements: 1) a stability measure, 2) Hebb-like mechanisms acting on the stabilities of pairs of synapses (each element in a correspondence detector pair is from this point onwards referred to as a synapse), 3) a neural trace and 4) random rewiring. These elements were chosen partly due to their practical significance and partly because of their biological relevance. In the following paragraphs we will describe each one of the model's main elements. Note that in a biological context the expression *learning algorithm* can, or should be, substituted by the expression *developmental process*.

The stability measure determines how likely a synapticpair (representing a particular correspondence detector) will be eliminated. The higher the stability value of a synaptic-pair, the less likely it is to be eliminated.

The stability measures of synaptic-pairs indirectly control how the patterns of connections between neurons are gradually molded. The question is then, what controls these stability measures? Our learning algorithm, which simulates a simplified developmental process, employs local Hebb-like mechanisms, which can be summarised by the following two rules: 1) when a synaptic-pair is active (i.e. the correspondence it represents is detected in the environment) and the postsynaptic neuron (i.e. a vode node to which it is connected) is also active, then the stability of that pair increases, 2) when the activity of a synaptic-pair and its postsynaptic neuron is decorrelated, the stability of the pair decreases. The mechanisms employed here exhibit two main differences relative to a conventional Hebbian synapse: 1) two synapses rather than one are involved in the process and 2) the changes caused by the learning rule do not affect the efficacy (see Hebb 1949) of the presynaptic neuron causing the postsynaptic neuron to fire (as in the notion of connection weights) but rather, affect the probability of the synaptic-pair being eliminated.

As already mentioned, in a Hebbian synapse correlated activity between pre and postsynaptic neurons increases the relevant connection strengths (see Havkin 1999 for a good introduction). A neural trace is essentially the prolonging of this effect throughout time. A modified Hebbian rule for example (Földiák 1991) might state that changes in synaptic strength are proportional to presynaptic activity and a temporal average of post-synaptic activity. As demonstrated in (Földiák 1991), neural traces are very useful for capturing invariant properties the environment. Interestingly, and maybe of unsurprisingly, the same mechanism that throws away transformation information for the implementation of invariant feature-detectors, is useful for the learning (or simulated development) of architectures that can detect/estimate those very same transformations. The idea is based on the notion that transformations are somewhat stable through time. If transformation Xoccurs between time t1 and time t4, and node n1 is activated at t1, then propagating some of n1's activity to the following time-step (similarly to a conventional neural trace), makes it more likely that n1 will be activated again for the same transformation X, thus accelerating the learning of "*n1* represents transformation X".

When synaptic-pairs are eliminated, new ones must be formed. Ideally, one would like the correct synaptic-pair to be generated, but again, we have to rely on "blind" local mechanisms. Thus random pairs of synapses are chosen for the substitution of eliminated correspondence detectors. The only exception to randomness employed assumes that the constituent synapses of any synaptic pair originate from different maps (i.e. one synapse from the source pattern and the other from the target pattern).

Algorithm 1 shows how the activities and stabilities of synaptic-pairs are updated. The algorithm begins by computing the activations of vote neurons as specified in Algorithm 2. Based on the neural activations computed via line 11 in Algorithm 2, Algorithm 1 then selects the node (i.e. win) with the largest activation, stores the latter's activity in wA and resets the non-winners to zero. Clearly, this is a simplification that warrants further elaboration in future experiments (e.g. iterative isolation of maximum values through lateral inhibition). The model also simplified the neural trace, which essentially consists of an upper bounded propagation of the winner's activity to the following iteration (see line 4 of Algorithm 2). Following this, Algorithm 1 proceeds to implement four Hebb-like rules (i.e. R1, R2, R3 and R4).

Algorith	m 1 Update Network State	
1:	procedure UPDATENETSTATE($net, IV_{old}, IV_{new}, p$)	
2:	$net \leftarrow compActivations(net, IV_{old}, IV_{new}, p)$	
3:	$Votes \leftarrow getVotes(net)$	
4:	$nS \leftarrow getNumSynpairs(Votes)$	
5:	$[win, wA] \leftarrow getWinner(Votes)$	
6:	$net \leftarrow resetLosers(net,win) > Activ. losers$	← 0
7:	$net \leftarrow makeTraces(net,win,p.maxTrace) \triangleright For net$	xt iter
8:	for all $v \in V$ otes do \triangleright Scan vote neu	rons
9:	for all $s \in getSynpairs(v)$ do \triangleright Synaptic p	Dairs
10:	If $v \neq win \& s.activ \equiv 0$ then	> K I
11:	If $s.stab \leq 0$ then	
12:	s.stab = s.stab - 0.5	
13:	end if $(1 - 1) = 1$	D 2
14:	else if $v \neq win \& s.activ \equiv 1$ then if	> K2
15:	$ s.stao \leq 1$ then $ $	R2.1
10:	$s.stab \leftarrow s.stab - 1$	D D D
17:	else	R2.2
18:	$s.stab \leftarrow s.stab - \alpha/s.stab$	
20:	end if $u = win & a activ = 1$ then $v = 1$	D 2
20.	erse if $v \equiv win \approx s.ucriv \equiv 1$ then if	× K5
21.	also if $v = win \ b \ c \ activ = 0$ then the	R4
22.	if s stab ≤ 1 then \Rightarrow	R/ 1
22.	$s \operatorname{stab} \leftarrow s \operatorname{stab} - 1$	104.1
21.	else b	R4 2
26.	$decr = (\alpha/s \ stab) + \beta(wA/nS)$	3)
27.	$s.stab \leftarrow s.stab - decr$	~)
28:	end if	
29:	end if	
30:	if $s.stab < p.minStab$ then \triangleright Stabil. 1	ims.
31:	s.stab = p.minStab	
32:	else if $s.stab > p.maxStab$ then	
33:	s.stab = p.maxStab	
34:	end if	
35:	end for	
36:	end for	
37:	end procedure	

Within the rules section of Algorithm 1, *s.activ* refers to the activity level of synaptic-pair *s* (*one* represents a detected correspondence while *zero* represents an undetected correspondence), *s.stab* refers to the stability of synaptic-pair *s*, which is limited by upper (i.e. *maxStab*) and lower (i.e. *minStab*) bounds. The four rules essentially represent all possible combinations between whether vote neurons are winners or not, and whether synaptic-pairs are active or not.

Algoritl	hm 2 Compute Activation	ons
1:	procedure COMPACTIVA	$fions(net, IV_{old}, IV_{new}, p)$
2:	$Votes \leftarrow getVotes(f)$	net)
3:	for all $v \in Votes$ do	▷ Scan vote nodes
4:	$v.activ \leftarrow v.trac$	$ce \triangleright Copy$ trace from previous iteration
5:	for all $s \in getSy$	$nPairs(v)$ do \triangleright Scan synaptic pairs
6:	$[S1, S2] \leftarrow g$	$etSynap(s) \mathrel{\triangleright} $ Individual synapses
7:	$F_{S1} \leftarrow IV_{old}$	$(S1_y, S1_x) $ \triangleright Source feature
8:	$F_{S2} \leftarrow IV_{net}$	$w(S2_y, S2_x) $ \triangleright Target feature
9:	if $F_{S1} \equiv F_{S2}$	then > Correspondence detected
10:	$s.activ \leftarrow$	− 1 ▷ Synpair activated
11:	$v.activ \leftarrow$	$-v.activ + 1 \triangleright$ Incr. vote activity
12:	else	▷ Correspondence not detected
13:	$s.activ \leftrightarrow$	− 0 ▷ Synpair inactivated
14:	end if	
15:	end for	
16:	end for	
17:	end procedure	

The environment simulation has one more function, apart from updating the attentional window and the network state, which should be mentioned, i.e.: *rewire*. This function essentially scans all synaptic-pairs in all vote nodes, and substitutes those synaptic-pairs whose measures of stability are smaller than some lower-bound, with new randomly chosen ones.

RESULTS

All of the experiments reported here were conducted in the context of constrained estimation, where the transformations of the attention window were restricted to horizontal and vertical shifts (i.e. two unknowns). Recall that correspondences are capable of constraining only two unknowns.

Refer to Figure 2 in order to get a better idea of how overall synaptic-pair stability changes with time. The yaxis (i.e. "percent stable") refers to the percentage of synaptic-pairs whose stabilities are larger than half of the maximum stability measure. The x-axis measures time in terms of simulation iterations. In order to remove the effects of extraneous factors, the graph averages the results of 5 simulations. In order to get a better understanding of the shape of this graph (e.g. why does learning slow down dramatically at later stages?), one must consider several probabilistic factors governing learning.



Since transformations change randomly, and the formation of synaptic pairs is also random, one can ask the following question: given a certain number of synaptic-pairs (regardless of the number of vote nodes) and given a particular range of transformations, what is the probability that at least one of the random synaptic-pairs matches the random transformation? Assuming constrained problems, in the case where there is no feature scarcity, the probability is defined by:

$$P(match) = 1 - \left(\frac{t-1}{t}\right)^s \tag{1}$$

where t represents the range of transformations that can occur and s represents the number of synaptic-pairs available.

Figure 3 depicts various curves representing different ranges of transformations for numbers of synaptic-pairs varying between 1 and 150.



It is important at this point to briefly describe the four main factors that make our learning problem difficult:

- 1. *Feature scarcity*. Environments which exhibit a small proportion of features, lead to low probabilities of correspondence detection, and thus to slow or even impaired learning.
- 2. *Feature repetition (or correlation).* The repetition of features leads to false correspondences (i.e. correspondences between matching features which nevertheless represent different object parts), which in their very nature are misleading and can therefore lead to erroneous connectivity.
- Guidance. How does each synapse from one map "know" which synapse it needs to pair up with from the other map? There is no global intelligence guiding the whole process, only local mechanisms.
- 4. Availability of correspondence detectors. The total number of possible inter-map conjunctions (or correspondences) is likely to be larger than what each neuron can represent.

Feature scarcity and repetition pertain to environmental issues whereas guidance and detector availability pertain to the neurobiological constraints mentioned earlier.

A synthetic image generator was devised in order to control feature scarcity. Figure 4 illustrates several learning curves under two conditions of feature scarcity, i.e.: low (on the left) and high (on the right). The graphs average the results of 20 simulations. Each graph consists of three curves: stability, T-Coverage (from transformation coverage) and C-Coverage (from correspondence coverage). The stability curve represents the percentage of synaptic-pairs with a stability value larger than half the maximum. The T-Coverage curve represents the percentage of environmental transformations represented by the network. If a particular transformation t is represented by a certain set of x correspondences and the synapticpairs of a particular vote node representing t detect x/2of that set, then the CCoverage for that vote node is 50%. The C-Coverage curve represents the average C-Coverages for all of the network's vote nodes.



Figure 4: Learning with different feature scarcities.

As predicted, when the environment manifested abundant features (left-hand side of Figure 4), learning proceeded seamlessly, with all three curves approximating 100%. When, on the other hand, feature scarcity was high (right-hand side of Figure 4), learning was somewhat hindered (i.e. both stability and C- Coverage curves stagnated at approximately 80%). Having said this, learning was better than expected, seeing that in spite of the scarcity of features, T-Coverage was capable of reaching 95% after about 5000 iterations. This is an indication that the learning algorithm is somewhat robust to feature scarcity.

Repeating (or correlated) features pose another problem to learning seeing that they lead to false correspondences, which by their very nature are misguiding. A synthetic image generator allowed us to control the number of repeating features in the environment. Figure 5 depicts the results from two conditions, defined by the image's average probability of a true correspondence (i.e. a correspondence between matching features which represent the same object part), which is a direct result of feature repeatability. The curves (stability, T-Coverage and C-Coverage) are defined in the same way as those in Figure 4 and represent averages from 20 simulations.

Both conditions allowed T-Coverage to approximate 100%. However, as the probability of a true correspondence (PTC) decreased from 0.7 to 0.53 the main victims were C-Coverage and learning speed. Regarding the latter, note that when PTC was 0.7, T-Coverage approximated 100% at about iteration *5,000*, whereas when PTC was 0.53, T-Coverage approximated 100% at about iteration *18,000*.



Although it is useful to verify the model's robustness to synthetic images with varying levels of feature scarcity and repeatability, ultimately the main question asks how it behaves in the context of natural images. As already mentioned, raw natural images are rich with features. Furthermore, and especially at local scales, natural images exhibit few feature repetitions and therefore lead to a small proportion of false correspondences. Figure 6(b) contains a graph depicting the mean PTCs and standard deviations of the natural image in Figure 6(a), for different local scales (window radii). The mean PTC for local scale x is computed by scanning the image with a window of radius x, computing the PTC of the window's data relative to itself, for each position, and then averaging the results. Notice how the mean PTC and its standard deviation are inversely proportional to window radius.



Figure 6: Several PTCs of a natural image.

The PTC of a window can be calculated using the following expression:

$$P(TC) = \frac{n + \sum_{i=1}^{r} x_i}{n + \sum_{i=1}^{r} (x_i)^2}$$
(2)

where *n* represents the number of non-repeating features, *r* represents the number of repeating feature types and x_i represents the number of elements exhibited by repeating feature type *i*. Thus, the numerator refers to the number of true correspondences provided by a particular window, while the denominator refers to the total number of correspondences (i.e. true and false correspondences).

Figure 7 confirms our optimism and demonstrates that learning proceeds quite effectively in the context of natural images. The simulation was programmed to stop at the overall stability level of 95%, at which point both the T-Coverage and C-Coverage curves both approximated 100%. As before, the curves were averaged from 20 simulation runs.



Figure 7: Learning in the context of natural images.

CONCLUSION

proposed neural This paper has architectures implementing the functionality of unsupervised clustering of correspondence detectors as a viable approach to the problem of pose estimation. Moreover, it has focused on purely local learning mechanisms which makes the approach relevant not only to applied domains but also to the simulation of biological systems. The experiments carried out thus far constitute useful proofs of concept and thus encourage several lines of future work.

The utility of correspondences, and thus the benefits of their unsupervised clustering, are not restricted to visual pose estimation (or even the visual modality). There are many other visual problems that can be solved via correspondences and thus, which warrant the same kind of study presented here, e.g.:

- 1. *Motion analysis*. The problem of motion analysis (or object tracking), as this paper has shown, can be formulated in terms of pose estimation between time frames.
- Stereopsis. The computation of disparity for stereopsis relies on finding *corresponding* features from both retinas, which in turn can be implemented by an architecture employing intermap conjunctions.
- 3. *Shape representation*. In (Osada et al. 2002), it was shown how a shape can be represented by the statistics of the distributions of correspondences occurring between the shape and itself.
- 4. *Edge orientation estimation*. Correspondences within an edge pattern can vote for particular orientations, thus calling for an architecture involving inter-map conjunctions and vote summation.

In another line of research it should be useful to relax the neurobiological constraints applied in this study and thus for example allow each vote-node to represent all possible correspondences. In this scenario. correspondences would no longer require a stability measure, and instead would use a firing efficacy measure (much like a traditional weight), which can be interpreted as a fuzzy membership function. It would be interesting to see how different network architectures might be capable of learning different kinds of efficient representations (e.g. can six vote nodes efficiently represent a space consisting of 100 different transformations, through the unsupervised learning of a broad tuning coding strategy?).

The results reported here demonstrate the application of correspondences with regards to a constrained problem (i.e. horizontal and vertical shifts). Although work has already begun in this direction, it would be interesting to further pursue the question of how the approach can be optimized with reference to unconstrained problems, i.e.: problems that involve more than two unknowns, such as similarity transformations (translation, rotation and scaling).

To conclude, we would also like to look into the question of how to prove (or disprove) the implementation of correspondence-based approaches in biological neural systems. Relatively recent work has made it clear that the computational machinery required to implement the approach efficiently does indeed exist in biological systems. Correspondence detection, for instance, can be computed by logical conjunctions implemented by non-linear computations taking place at local regions of dendritic trees (Polsky et al. 2004), whereas vote nodes can be implemented by traditional signal integration processes. Recent neurohistological methods (Gan et al. 2000; Grutzendler et al. 2003) might provide the means to prove (or disprove) our hypothesis. In these methods, multiply colored dyes are applied to neural tissue via particle-mediated ballistic delivery, fully staining neurons in a Golgi-like manner. If it is possible to identify and target two neuronal maps and apply differently colored labels to them, then it should be possible to deduce some of the computations taking place between them by observing the colors and placements of synapses at their target locations (see Figure 8 for a simplified illustration).





Figure 8: Visualization of inter-map conjunctions.

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CO-EVOLUTIONARY LEARNING OF CONTEXTUAL ASYMMETRIC ACTORS

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KEYWORDS

Repeated encounter games, asymmetric payoff, coevolutionary learning, multi-population, spanish democratic transition.

ABSTRACT

Co-evolutionary learning of the iterated prisoner's dilemma (IPD) has been used to model and simulate interactions, which may not be realistic due to assumptions of a fixed and symmetric payoff matrix for all players. Recently, we proposed to extend the co-evolutionary learning framework for any two-player repeated encounter game to model more realistic behavioral interactions. One issue we studied is to endow players with individual and self-adaptive payoff matrix to model individual variations in their utility expectations of rewards for making certain decisions. Here, we study a different issue involving contextual asymmetric actors. The differences in the utility expectations (payoff matrix) are due to contextual circumstances (external) such as political roles rather than variations in individual preferences (internal). We emphasize the model of interactions among contextually asymmetric actors through a multi-population structure in the co-evolutionary learning framework where different populations representing different actor roles interact. We study how different actor roles modelled by fixed and asymmetric payoff matrices can have an impact to the outcome of co-evolutionary learning. As an illustration, we apply co-evolutionary learning of two contextually asymmetric actors from the spanish democratic transition.

INTRODUCTION

The iterated prisoner's dilemma (IPD) has become the standard metaphor to explain cooperative behaviors among selfish, unrelated individuals (Axelrod, 1984). In its classical form, two players are given two choices, cooperate and defect, and engaged in repeated interactions. The game captures the *dilemma* of cooperative interactions between unrelated, selfish players seeking the highest payoffs through the payoff matrix that defines rewards players received based on the joint choices they made in a behavioral exchange. Although payoffs for mutual cooperation are higher compared to that of mutual defection, a player that exploit its opponents will receive the highest payoff while the opponent receives the lowest payoff.

However, defection is not always the best choice for the IPD. Axelrod (Axelrod, 1980a,b) showed through tournaments of experts-designed strategies that a particular form of cooperative strategy, tit for tat, that cooperates in the first round and reciprocates thereafter the choice that the opponent made, can be viable. Other studies (Axelrod, 1984; Nowak and Sigmund, 1992) have explained cooperation in the IPD using the notion of reciprocal altruism. i.e., cooperative behaviors arises from repeated encounters that allows cooperation received by an individual to be returned. Further studies have formulated and shown that co-evolutionary models (Axelrod, 1987; Fogel, 1991, 1993; Darwen and Yao, 1995; Julstrom, 1997; Chong et al., 2007) allow cooperative behaviors to be learned through an adaptation process on behavioral representation guided by strategic interactions.

It is noted that all of these studies have assumed that the utility expectation on rewards (payoff matrix) of a strategy for making certain decisions does not change (fixed) and is similar for all strategies (symmetric). These two assumptions may not be realistic if the IPD is used as a model to explain outcomes of real-world interactions due to variations between individuals, which are reflected by them having different utility expectation (payoff matrix) (Johnson et al., 2002). Cooperative outcomes may be due to a different payoff matrix that favors mutual cooperation (i.e., mutualism (Clements and Stephens, 1995)).

Recently, we (Chong and Yao, 2006) proposed to extend the co-evolutionary learning framework for any twoplayer repeated encounter game that address the restrictive assumptions of having fixed and symmetric payoff

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matrix, and allows the modelling of more realistic behavioral interactions. One issue we studied is to endow players with individual and self-adaptive payoff matrix to model individual variations in their utility expectations of rewards for making certain decisions. The result of the co-evolutionary process is that the evolutionary outcome is dependent on the adaptation process of both behaviors (strategy behavioral responses) and utility expectations that determine how behaviors are rewarded (strategy payoff matrices).

In this paper, we study a different issue involving contextual asymmetric actors. The differences in the utility expectations (payoff matrix) are due to contextual circumstances (external) such as political roles rather than variations in individual preferences (internal). The model of interactions among contextually asymmetric actors are achieved using a multi-population structure in the co-evolutionary learning framework. With the single-population framework (Chong and Yao, 2006), strategies undergoing evolutionary (selection and variation) processes in the same population can only represent actors that are contextually similar in roles, despite their variations in individual payoff matrices. With the multi-population framework, the evolution of strategies within a population is guided by strategic interactions with strategies in other populations. This allows the modelling of behavioral exchange between contextually asymmetric actors as different populations represent different actor roles.

We study and show how different actor roles modelled by fixed and asymmetric payoff matrices can have an impact in the co-evolutionary learning of behaviors through empirical studies. As an example, we show that the coevolution of a population using IPD payoff matrix that interacts with another population using mutualism payoff matrix can lead to mutual cooperation. Mutual cooperation is achieved if rewards for exploitation are sufficiently low. In another example, we consider a real-world political setting through the study of the co-evolutionary learning of two dissimilar actor roles, Franco (dictator) and Juan Carlos (prince), where results suggested that the circumstances of Franco and Juan Carlos learning to mutually cooperate are a result of Juan Carlos reflecting Franco's favorable expectation of a suitable successor.

The rest of the paper is organized as follows. The following section describes the general setting for iterated, two-player, two-choice games to model behavioral interactions. After that, a literature background for the case study on the Spanish Democracy Transition is provided. The following section then describes the co-evolutionary framework used for the experiments in detail. Results of the experiments are then reported with discussions on the observations obtained from the experimental results. Finally, the paper finishes with conclusion with some remarks for future studies.

REPEATED ENCOUNTER GAMES

Repeated encounter games have been used generally to model behavioral interactions. One example is the symmetric, two-player, two-choice game as a model for cooperation (Mesterton-Gibbons and Dugatkin, 1992). Here, each players have the choice of either to cooperate or defect. Depending of the choices that both players have made, each player receives a payoff that is specified by a predefined payoff matrix (Fig. 1). Both players receive R units if both cooperates, or P units if both defects. However, if one player cooperates while the other defects, the cooperator will receive S units while the defector receives T units. The values R, S, T, and P must satisfy the constraints, R > P and R > (S + T)/2. Note that for Figure 1, the payoff given in the lower lefthand corner is assigned to the player (row) choosing the move, while that of the upper right-hand corner is assigned to the opponent (column). The game is said to be symmetrical if the payoff matrix is the same for both players (Mesterton-Gibbons and Dugatkin, 1992).

	Cooperate	Defect
	R	Т
Cooperate		
	R	S
	S	Р
Defect		
	Т	Р

Figure 1: The Payoff Matrix Framework of a Two-Player, Two-Choice Game

Games with different characteristics can be produced depending on the specifications for R, S, T, and P. For example, in a simple single iteration game, when T > R > P > S, one obtains the prisoner's dilemma game, where the best choice is to defect. However, when R > T and S > P, one obtains the mutualism game, where the best choice is to cooperate (Clements and Stephens, 1995). Both of these games can be extended to have more than one iteration in the form of iterated games to model repeated encounters (Johnson et al., 2002).

In (Chong and Yao, 2006), we proposed a generic framework of repeated encounter games, whereby the payoff matrix is different and adaptable for each strategy. The framework is applicable to any repeated encounter game with different payoff matrices, and not just limited to those that satisfy specific constraints such as the IPD or mutualism games.

SPANISH DEMOCRATIC TRANSITION

The Spanish transition to democracy (1975-1982) is a period of significance and interest as it uniquely demonstrates the capacity to transform a right wing dictatorship of Francisco Franco to a socialist government of Felipe González in a period of seven years, marking it as the only transition of its kind in history (Figure 2). Much has been written in terms of historical discussion but little in the regard of scientific analysis of the actions taken. In particular, the necessity to understand on a more fundamental level the capabilities and constraints associated with individual involvement in democratic transitions is intricately connected to a comprehensive awareness of the form of transitions as a process (Hill, 2007).

1936 – 1939	Spanish Civil War
1938, Jan 5th	Birth of Juan Carlos in Rome
1939, Apr 1st	Franco defeats Republican forces
	and takes control of Spain
1969	Franco designates Juan Carlos as
	heir – no real power endowed
1975, Nov 20th	Death of Franco
1975, Nov 22nd	Juan Carlos crowned King of Spain
1982	Socialist Party elected to power

Figure 2: Spanish Democratic Transition Timeline

Throughout the transition period Franco held the dominant position, effecting change and directing the order of progression. The primary objective of the dictator lay in his desire to ensure the survival of his regime after his death and the manner in which he chose to effect this was through the creation of a francoist monarchy. In terms of pure power distribution, Juan Carlos was very much the subservient player even though his interests converged with those of Franco. The desired result would culminate for both men in the nomination of Juan Carlos as King of Spain and the guaranteed continuation and prosperity of the existing regime.

Franco's desire for a francoist monarchy is evident by his actions regarding Juan Carlos. The desire for legitimacy (Gilmour, 1985), as represented by Juan Carlos' bloodline, outweighed any previous evidence of the dictator's animosity towards the young prince's family. Franco called Juan Carlos back from exile in order to establish a dynasty that would sustain his vision for Spain. Franco had allowed Juan Carlos to return to Spain under very specific conditions, with his education and upbringing closely monitored. Juan Carlos was provided scarce opportunity to be anything other than that which Franco required. Franco saw this as the mechanism to ensure continuation of his rule and Juan Carlos believed this as the only manner by which a Borbón (prior royal family) would once again inherit the throne. Franco needed a successor, and Juan Carlos had both the lineage and the ability to create what Franco had been unable to; a francoist monarchy. However, Juan Carlos was aware even at this stage that the only way to gain access to the throne was through Franco (Cernuda, 1981) and the dangers inherent in acting against him (Hill, 2007).

As illustrated in Table 1, Juan Carlos (JC) represented

Table 1: Payoff Matrix	Scenario fe	or Spanish	Democratic
Transition			

	SCENE1		SCENE2		SCE	NE3
	FC	JC	FC	JC	FC	JC
R	1	1	1	1	0	1
S	0	-1	0	-1	-1	-1
T	0	-1	0	-1	1	-1
P	-1	-1	0	-1	1	-1

the ideal choice for Franco (FC) under ideal circumstances (SCENE1) but alternative solutions could be generated based upon a reordering of individual preferences or a more fundamental understanding of relative gains that are made possible simply because of the power Franco had. Deviation on the part of Juan Carlos (Gibson, 1992) and an awareness of alternative choices on the part of Franco would lead to a situation whereby Franco's ideal preference would remain that of Juan Carlos but he would be prepared to accept an alternative candidate if forced to. Juan Carlos on the other hand, would remain powerless to effect change given the emergence of an alternative for Franco (reflected by the reduction of rewards for P in SCENE2 for FC's payoff matrix while no changes are made to JC's payoff matrix) (Hill, 2007).

Under the scenario listed above, the choice of Juan Carlos was an artificial constraint generated by Franco's desire for legitmacy and monarchy (Gunther, 1992). The nature of this constraint equally depended upon the character and actions of Juan Carlos and therefore endowed Franco with the ability to alter the status quo by reordering his preferences should the actions of Juan Carlos deviate from expectations. If legitimacy and legacy could be achieved without royal blood (Alba, 1978) then the choices available to Franco would change considerably even if those available to Juan Carlos are unaffected (SCENE3).

In analyzing the Spanish transition to democracy, despite Franco's selection of Juan Carlos, we cannot conclude that he constituted the only choice. Franco's ability (outlined by the Law of Succession) to remove Juan Carlos indicates that we must be cautious about any assumptions we make. It became imperative for Juan Carlos to retain Franco's trust and patronage, as this would enable consolidation of his own position and potential for future development. Providing the decisions taken could not be enforced by a third party (e.g., the military) (Powell, 1991), Juan Carlos would be in an advantageous position upon accepting the nomination. The power and influence he gained through his association with Franco would grant him a measure of freedom but the all-important factor became, assuring that he received the nomination at all.

CO-EVOLUTIONARY LEARNING

Strategy Representation

We limit our investigations to only deterministic, memory-one strategy for simplicity. We consider the same direct look-up table strategy representation proposed and studied earlier in (Chong and Yao, 2005), which allows direct behavioral evolution of strategies. Figure 3 illustrates this strategy representation. m_{ij} , i, j = 1, 2 specifies the choice to be made, given the inputs *i* (player's own previous choice) and *j* (opponent's previous choice). Instead of using pre-game inputs (two for memory-one strategies), the first move is specified independently, m_{fm} . Binary choices of +1 and -1are used to represent cooperate and defect, respectively.

		Opponent's Previous Move	
		+1	-1
Player's	+1	m_{11}	m_{12}
Previous Move	-1	m_{21}	m_{22}

Figure 3: The Look-Up Table Strategy Representation for the Two-Player Repeated Encounter Game with Two Choices and Memory Length One

A simple mutation operator is used to generate offspring from parents. Mutation replaces the original element with the other possible choice. For example, if mutation occurs at $m_{11} = +1$, then the mutated element m'_{11} takes -1. Each table element has a fixed probability, p_m , of being replaced by the other choice. The value p_m is not optimized, and crossover is not used in any of the experiments as mutation alone is sufficient to introduce variations to strategy representation.

Co-evolutionary Learning Procedure

We describe in detail an example of a multi-population co-evolutionary learning framework to model behavioral interactions of contextually asymmetric actors. The two-population co-evolutionary learning allows the adaptation of strategy behavioral responses. The twopopulation co-evolutionary learning procedure is described as follows:

1. Generation step, t = 0:

Initialize N/2 parent strategies in the first population, $P_i^1, i = 1, 2, ..., N/2$, and in the second population, $P_i^2, i = 1, 2, ..., N/2$, randomly. Each table element, m_{fm} and $m_{ij}, i, j = 1, 2$, is initialized to values, +1 or -1, each with equal probability.

2. Generate N/2 offspring, $O_i^1, i = 1, 2, ..., N/2$, from N/2 parents, $P_i^1, i = 1, 2, ..., N/2$, for the first population and N/2 offspring, $O_i^2, i = 1, 2, ..., N/2$, from N/2 parents, $P_i^2, i =$ 1, 2, ..., N/2, for the second population using a mutation operator with probability $p_m = 0.05$.

- 3. Each strategy in the first population compete with each strategy in the second population (i.e., full-mixing, where for N strategies in a population, every strategy competes a total of N games).
- 4. Select the best N/2 strategies based on total payoffs of all games played for both populations. Increment generation step, t = t + 1.
- 5. Step 2 to 4 are repeated until termination criterion (i.e., a fixed number of generation) is met.

For the experiments, we use N = 20 and repeat the coevolutionary process for 200 generations, which is sufficiently long to observe an evolutionary outcome (e.g., persistent cooperation). A fixed game length of 150 iterations is used for all game. Experiments are repeated for 30 independent runs.

We note the fundamental difference between the multipopulation co-evolutionary learning framework and the single-population frameworks studied earlier such as in (Chong and Yao, 2005, 2006). Considering the singlepopulation framework in (Chong and Yao, 2006), strategies undergoing evolutionary processes in the same population can only represent actors that are contextually similar in roles, despite their variations in individual payoff matrices. For the two-population co-evolutionary learning that we study here, strategies undergo evolutionary processes within their own populations (i.e., strategies from the first population will not be mixed with and transferred to the second population, and vice versa). Furthermore, the co-evolution of strategies in the first population will be guided by the results of interactions with strategies from the second population, and vice versa. This allows the modelling of behavioral exchange between contextually asymmetric actors as different populations represent different actor roles.

We also note other forms of mutiple-population coevolutionary learning framework such as cooperative coevolution Potter and Jong (2000). However, the motivation for having a multi-population framework in cooperative co-evolution is to have samples of different subcomponents undergoing evolutionary processes that can later be combined to obtain the full solution (i.e., divideand-conquer). Here, the multi-population framework is applied to a competitive co-evolution approach where the motivation is to have solutions (strategies) competing with one another through interactions (game-play).

RESULTS AND DISCUSSION

Learning Behaviors For Contextually Asymmetric Actors

We start our study by first investigating the impact of having contextually asymmetric actors to the behavioral outcomes of the two-population co-evolutionary learning. For baseline comparison, we first consider the case where the payoff matrices for each strategy are fixed and the same. As an example, we consider both populations with the same IPD payoff matrix. Note that we label an experiment as [First Population Payoff Matrix]-[Second Population Payoff Matrix]. For example, IPD1-IPD1 refers to the experiment where the first and second populations use an IPD payoff matrix as shown in Table 2. We use IPD1-IPD1-P1 and IPD1-IPD1-P2 to refer to the evolutionary outcomes of the first and second population, respectively.

 Table 2: Payoff Matrix Labels for Repeated Encounter

 Games

	IPD1	IPD2	MUT
R	4	4	5
S	0	0	1
T	5	6	4
P	1	1	0

It is noted that a two-population structure is imposed to the co-evolution whereby strategies undergo evolutionary processes in their own respective populations. However, the evolved strategies between the two populations interact with one another through IPD game-plays. As such, we would expect that evolved strategies would learn to play cooperatively through co-evolution starting from random initialization, which is the outcome one would observe from a single-population co-evolutionary learning (Chong and Yao, 2005). Experimental results show that the majority of runs ended with cooperative outcomes (Table 3), which one can further observe from the higher percentages of cooperation being played on average (i.e., more than 50%) (Table 3).

Table 3: Experimental Result for Number of Runs where "No < 25%" Indicates Majority Play is Defection while "No > 75%" is for Cooperation

	No < 25%	No > 75%
IPD1-IPD1-P1	4	24
IPD1-IPD1-P2	4	24
IPD1-MUT-P1	8	22
IPD1-MUT-P2	0	30
IPD2-MUT-P1	12	17
IPD2-MUT-P2	0	29

However, the payoff matrices for both populations need not be the same. We investigate the case of a population with the IPD payoff matrix (IPD1) and the other population with the iterated mutualism payoff matrix (MUT). Although one would expect both populations learning to cooperative (Table 3), the second population using MUT would play more cooperatively as shown by the increase in the number of runs having cooperative outcomes (Table 3) and an increase of cooperation plays that is statistically significant (Table 4). When the first population uses an IPD payoff matrix that further rewards strategies that are tempted to defect and exploit oppo-

Table 4: Experimental Results for Average of Cooperation Frequency over 30 Runs in % with a Confidence Interval of 95% in % and *t*-test where [†] Indicates a Statistical Significant Difference

0					
	Mean \pm Std Err	t-test			
IPD1-IPD1-P1	77.09 ± 11.71				
IPD1-IPD1-P2	78.85 ± 11.88				
IPD1-MUT-P1	70.33 ± 14.87	0.78			
IPD1-MUT-P2	95.85 ± 1.10	-2.82^{\dagger}			
IPD2-MUT-P1	42.38 ± 16.54	3.32^{\dagger}			
IPD2-MUT-P2	94.36 ± 3.27	-2.43^{\dagger}			

nents (IPD2), results show that the first population would learn to play significantly less cooperative (Tables 3 and 4) although the second population still plays significantly more cooperative as a result of MUT payoff matrix. Finally, we observe that all populations that learned to cooperate converged to a stable and high cooperative plays compared to the population that did not learn to cooperate, which exhibited fluctuations during co-evolution.

Although results coincide strongly with our expectation on the outcome of co-evolutionary learning given how payoff matrices are assigned to the two populations, these investigations further highlight the subtle but important differences between a multi-population and single-population co-evolutionary learning framework to model behavioral interactions. In particular, the twopopulation co-evolution made it possible to study the learning of behavioral responses between two contextually asymmetric actors having different utility expectations to rewards for the same joint actions.

Co-evolutionary Analysis Of The Spanish Democracy Transition

In this section, we study the two-population coevolutionary learning framework applied to model the Spanish Democratic Transition. Although historical outcome of the interactions between the two actors, Franco (dictator) and Juan Carlos (Prince), is known and that various political science arguments have been given to explain the cooperative outcome leading to the transition, it is not really known why they have chosen to cooperate. Here, we study and offer an analysis to the Spanish Democratic Transition through co-evolutionary learning. We assume that the two actors are rational beings (seeking to maximize payoffs) and capable of learning behavioral responses based only on interactions with one another. In using the two-population co-evolution, the first and second populations will represent samples of behaviors for Franco and Juan Carlos, respectively. We consider the payoff matrices for the populations representing Franco (PFC) and Juan Carlos (PJC) based on possible scenarios identified earlier (Hill, 2007) and listed in Table 1.

Tables 5 and 6 summarize the results of the experi-

Table 5: Spanish Democratic Transitions: Experimental Result for Number of Runs where "No < 25%" Indicates Majority Play is Defection while "No > 75%" is for Cooperation

	No < 25%	No > 75%
SCENE1-PFC	0	30
SCENE1-PJC	0	30
SCENE2-PFC	0	30
SCENE2-PJC	0	30
SCENE3-PFC	30	0
SCENE3-PJC	0	24

Table 6: Spanish Democratic Transitions: Experimental Results for Average of Cooperation Frequency over 30 Runs in % with a Confidence Interval of 95% in % and *t*-test where [†] Indicates a Statistical Significant Difference

	Mean \pm Std Err	t-test
SCENE1-PFC	98.16 ± 0.87	
SCENE1-PJC	97.10 ± 1.54	
SCENE2-PFC	97.42 ± 1.16	1.43
SCENE2-PJC	96.90 ± 1.43	0.56
SCENE3-PFC	3.59 ± 1.34	108^{\dagger}
SCENE3-PJC	87.70 ± 6.59	3.02^{\dagger}

ments for the modelling of Spanish Democratic Transition scenario. For SCENE1 and SCENE2 experiments, both populations evolve to mutual cooperation play starting from random initializations of strategy behaviors. Although results suggest that strategies representing Franco and Juan Carlos learn to cooperate with the political succession (e.g., no statistical differences in the outcomes of cooperative plays), one needs to note the subtle difference between the two scenario that represents different conditions with which mutual cooperation is learned. In both scenario, the payoff matrix of Juan Carlos (Table 1) reflects his expectation that he is not the only available successor, in which case, he is better of cooperating. However, the payoff matrix of Franco for the two scenario differs, i.e., SCENE1 reflects the case that Franco wants Juan Carlos to succeed while SCENE2 reflects the case that Juan Carlos represents the ideal choice but other alternatives are considered (lower P for the case of SCENE2 compared to that of SCENE1).

Results for SCENE1 and SCENE2 are in agreement with the historical outcome of the Spanish Democratic Transitions, suggesting that Franco would have wanted Juan Carlos to succeed. However, what if there are other equally suitable alternatives that are within Franco's expectation. SCENE3 reflects one possibility that the royal lineage of Juan Carlos is not necessarily the important factor in the succession and that Franco has the political power to choose other alternatives. In this case, our experimental results suggest that mutual cooperation is not possible, i.e., that strategies representing Franco would learn to defect (choosing another successor) despite cooperation from strategies representing Juan Carlos.

CONCLUSION

This paper has studied behavioral interactions involving contextually asymmetric actors. The main motivation is to address the issue that real-world interactions involving actor roles that are contextually different. We modelled behavioral interactions of contextual asymmetric actors through a multi-population co-evolutionary learning framework. Unlike the single-population framework where strategies only represent contextually similar actor role, the multi-population framework models behavioral exchange between contextually asymmetric actors with different populations representing different actor roles, with co-evolution guided by strategic interactions with strategies between populations.

We showed that different actor roles modelled by fixed and asymmetric payoff matrices can have an impact in the co-evolutionary learning of behaviors through empirical studies. In one example, we showed that the coevolution of a population using IPD payoff matrix that interacts with another population using mutualism payoff matrix can lead to mutual cooperation if rewards for exploitation are sufficiently low. In another example, we studied a real-world political setting of the Spanish Democratic Transitions, where results suggested that the circumstances of Franco and Juan Carlos learning to mutually cooperate are a result of Juan Carlos reflecting Franco's favorable expectation of a suitable successor.

This paper presents a preliminary study on behavioral interactions involving contextually asymmetric actors. Future studies would investigate other issues involving more complex interactions in political transitions.

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MULTI-RESOLUTION OPTIMISATION: APPLICATION OF META-HEURISTIC IN FUNCTION REMODELLING

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KEYWORDS

Optimisation, Function Remodelling, Meta-Heuristic, Approximation, Estimation, Smoothing.

ABSTRACT

Multi-resolution approach to optimisation involving remodelling of objective function has great received interests lately. There are two different goals of remodelling for the objective function. First, the reduction of computational complexity of the objective functions in order to accelerate the searching process. Second, the removal of local optima in the objective functions to avoid premature convergence. Most of the approach shares the problem: the setting of the smoothness pressure value over the objective function. We proposed a meta-heuristic approach to determine the suitable smoothness pressure value throughout the searching process. The results show that meta-heuristic has significant improvement compared to state-of-theart Classic Evolutionary Programming (CEP) and Fast Evolutionary Programming (FEP).

INTRODUCTION

Continuous Optimisation is a non-linear programming problem that involves finding the optimal solution in a given solution space. Often, the form of optimisation is defined as an objective function, which determines the fitness of given solution (Goldberg 1989; Lange 2004). A solution is defined as a vector or a set of real values. If the problem is bounded, the values are restricted in the lower bound and upper bound of the problem. Such as follow:

$$\min_{x_i \in X} f(x) = that \forall x' \neq x, f(x') > f(x)$$

$$where x, x' \in X and X \subset \mathbf{R}^N$$

$$low_i < x_i < high_i$$

$$(1)$$

The application of Evolutionary Algorithm (EA) in optimisation received attention due to their stochastic characteristic and capability of escaping local optima in the solution space (Goldberg 1989). Two issues that always surrounded by EA are the convergence speed and the quality of converged solution. Several algorithms that are based on EA have been proposed. These includes Memetic Algorithm (Krasnogor 2002), Cooperative Co-Evolutionary Algorithm (Popovici and Jong 2006). Other researches include improving the three major components of EA, which are the problem representation, selection and variation methods. Recently, variation method with higher probabilities of escaping local optima have been studied, such as Cauchy Mutation (Xin et al. 1999), Levy Mutation (Chang-Yong and Xin 2004), both producing promising results over benchmark testing functions.

On the other hand, improvement on problem representation is the remodelling of objective function. There are two different types of remodelling the objective function. First, the reduction of computational complexity of the objective functions in order to accelerate the searching process. Several regression techniques have been proposed, such as polynomial regression (Branke and Schmidt 2005), Gaussian/Kriging regression (Ratle 1998, 1999; Buche et al. 2005; Nakayama et al. 2001), these techniques have been implemented in Memetic Algorithm as local surrogates model for local searches (Zhou et al. 2007).

Second, the removal of local optima in the objective functions to avoid premature convergence. Techniques implemented in 2nd type includes: Polynomial (Quadratic) Approximation (Liang et al. 2000), Gaussian Kernel Smoothing (Yang and Flockton 1995), Truncated Fourier Series (Wang 2004). These techniques work under the condition that the remodelled function provides correct smoothness and certain degree of similarity compared to the objective function. As concluded by Liang et al, the Quadratic Approximation model performs worst than without remodelling if the problem does not carry quadratic characteristic (Liang et al. 2000). Gaussian Kernel Smoothing shares the same problem which the kernel size affects the smoothness of the remodelled function. Dekun Yang et al proposed a coarse-to-fine mechanism, where the kernel size reduces according to the searching progress. Bernardetta Addis et al discussed the same problem in (Addis et al. 2005) where Gaussian Smoothing Kernel is used together with numerical optimisation. In this paper, we further the investigation of the effect of Gaussian Smoothing

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) Kernel in optimisation, and proposed a metaheuristic approach in choosing the kernel size which reacts according to the current population.

BACKGROUND STUDY

Noise reduction is always an interesting issue in signal/image processing. The main purpose of noise reduction is to filter the unwanted signals that are caused by external factors. Local optima in optimisation share this characteristic, where the solution's fitness does not reflect the actual distance from optimal solution. To smooth continuous signals, a convolution transformation has to be done. As depicted in (Yang and Flockton 1995), the convolution transformation, or the approximation of function *f* is the integration of multiplication of smoothing kernel and the function. Let F_{β} be the approximated function with β as the smoothness pressure.

$$F_{\beta}(x) = \int_{y \in \mathbb{R}^{N}} h_{\beta}(y) f(x - y) dy$$
(2)
where h(y) satisfied $\lim_{\alpha \to 0} h_{\beta}(y) = \delta(y)$

Gaussian function satisfied condition in (2) and is given as below:

$$h_{\beta}(x) = \frac{1}{(2\pi)^{N/2} \beta^{N}} \exp(-x^{T} x/2\beta^{2})$$
(3)

The β and N are the kernel size and number of dimension respectively. That is, the higher the β , the smoother the approximated function. As Evolutionary Algorithm treats the optimisation as a black box searching process, the convolution of the function itself is prohibited. However, statistical learning suggested that if the sample size is large enough, then the convolution yields the similar result as the expected value (mean) of the fitness value of neighbour solutions. These solutions are sampled randomly according to the probability of Gaussian distribution, as depicted as y in (4).

$$F_{\beta}(x) = E_{\nu}[f(x-y)]$$
(4)

And the expected value of these neighbour solutions is its sample mean:

$$F_{\beta}(x) = \frac{1}{M} \sum_{i=1}^{M} f(x - y_i)$$
(5)

with y_i is randomly selected according to Gaussian distribution with β as the standard deviation. (2) to (5) are summarized from Dekun Yang et al (Yang and Flockton 1995). As discussed above, the β is the smoothness pressure of the approximated function. The β has to be carefully selected because if it is too small, the approximated function does not remove the local optima, whereas if it is too high, it removes the global optimum as well (Yang and Flockton 1995). In (Yang

and Flockton 1995), a coarse-to-fine mechanism is used, where β is arbitrary set to 3.0 initially and reduced 30% every eighty generation. First, the coarseto-fine mechanism does not reflect the underlying optimisation problem. Second, the approximated function F_{β} does not guarantee to have the same global optimum as original fitness function F, this is shown in figure 1, where β =3.0 and 2.0 shifted the global optimum of the function. This is referred as "curse of uncertainty", a term was coined in (Ong et al. 2006). It indicates that the improper approximation causes the local search returns non-local-optimum solution in F, but the solution appears to be local optimum in F_{β} . In fact, the smoothed function only provides the "area of interest" where there no local optima. Consider figure 2 and 3. Figure 2 suggested that the smooth function removed local optima while the global optimum remains. However, the finer interval in figure 3 shows that the global optimum in objective function remains in single point while the approximated function does not carry any optimum. Thus, the approximated function should only provides the "area of interest" while the actual searching process continues with solutions found in the approximated function.





Fig 3. Ackley with finer interval between -1 to 1.

METHODOLOGY

From the hyperheuristic/metaheuristic point of view, the approximated functions with different smoothness are different heuristics for solving the problem. Choosing the good approximation may result significant improvement on the algorithm, which includes faster convergence speed and better converged solution. A heuristic is informal action used in solving problem, often is cheap in computation complexity and yet a natural way of solving the problem(Cowling et al. 2002). A hyperheuristic is a heuristic that chooses low level heuristic independent from problem, such as CPU execute cycles, improvement of a consecutive heuristic, etc(Kendall and Soubeiga 2002; Cowling et al. 2002). Metaheuristic is a hyperheuristic but the choosing function is often problem dependent (Cowling et al. 2002), such as pre-clustering of class of problem and choose corresponding heuristic according to the problem class (Ong and Keane 2004).

Approximated function F_{β} should be balanced between the smoothness and the similarity. Smoothness is referred to the number of local optima in the searching space. It can be represented by the inverse of roughness. However, there is no other way to quantify local optima in the function except by finding all of them. Fortunately, the fluctuation of the function also reflects the number of local optima. The fluctuation of the function is associated with the standard deviation of itself, $\sigma(F)$.

roughness of
$$F \propto$$
 fluctuation of $F \propto \sigma(F)$ (6)

$$\mu = \int x F(x) dx \tag{7}$$

$$\sigma(F) = \sqrt{\int (x - \mu)^2 F(x) dx}$$
(8)

Similar to (2), the integration is prohibited, and can be replaced with unbiased estimator with uniform sampling:

$$\overline{x} = \frac{1}{N} \sum_{i=1}^{N} x_i \tag{9}$$

$$\sigma(F) = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})^2}$$
(10)

Similarity is referred here to the difference between the global optimum in F_{β} and F. Also, this cannot be assessed as the searching process does not know the actual global optimum in the searching space. However, the area difference between F_{β} and F may reflect the similarity as well. Thus, the comparison of the area of the underlying function is defined as $\lambda(F)$, which is normalised from root mean square error "*rmse*" from (Ong et al. 2006):

area difference
$$\propto \lambda(F_{\beta})$$

$$\lambda(F_{\beta}) = \frac{\|\int F_{\beta}(x) - F(x)dx\|}{\int F(x)dx}$$
(11)
for $\beta \in \mathbb{R}^{+}$

Followed by an unbiased estimator with uniform sampling:

$$\lambda(F_{\beta}) = \frac{\|\sum_{i=1}^{N} F_{\beta}(x) - F(x)\|}{\sum_{i=1}^{N} F(x)}$$
(12)

In order for (9-10), (12) to estimate the roughness and area difference between the approximated and objective function accurately, sample size N must be very large. Fortunately, the sample size can be reduced if the quantifying process only takes place for the current searching area, which are the solutions in the current population. Let p be the current population, and I_{best} and I_{worst} be the best and worst solution in population p. The current searching space is defined as γ , with abbreviation γ (i) indicate value of ith element:

for min problem

$$y(i) = \{x \in \mathbb{R} \mid I_{best}(i) < x < I_{worst}(i)\}$$
for max problem

$$y(i) = \{x \in \mathbb{R} \mid I_{best}(i) > x > I_{worst}(i)\}$$
(13)

The uniform sampling processes for (8) and (12) are performed within γ . The empirical model for the metaheuristic in choosing F_{β} out of a predefined set $\beta = \{\beta_1, \beta_2, \beta_3, ..., \beta_n\}$ is the β value that produce the minimum output of M(β):

$$M(\beta) = \alpha \sigma(F_{\beta}) + (1 - \alpha)\lambda(F_{\beta})$$
(14)

Where α is the weight associate with the roughness and area difference for each approximated function F_{β} . In this paper we select α value as 0.3. The authors are aware that $M(\beta)$ is a multi-objective optimisation problem. We avoid using multi-objective optimisation in this event due to the demonstration here is not about to choose the exact β but to estimate the good balance between smoothness and similarity.

The proposed algorithm is outlined in pseudo code in Fig 4. The procedure starts by randomly generates solutions into the population. To determine which approximation function F_{β} to use, the algorithm has to choose the suitable β , which M(β) evaluates all beta values and returns the suitable β . There are two phase in the searching process. The first phase search in F_{β} and when it convergence condition is met, the process continues on the second phase, which searches in F. The convergence condition we experimented is the number of generation without improvement, and it is set to two hundred generations.

Define Population as pop
Populate pop
Initialize Beta = $\{3.0, 2.0, 1.0, 0.5, 0.3, 0.1\}$
Initialize mutation rate=3.0
Initialize generation=1
Choose B from Beta based on $M(\beta)$
Evaluate pop based on F_{β}
While(termination condition)
DO
set improvement=0
While(i < population size)
DO
Select individual i from pop
offspring = GaussianMutation(i, mutation rate)
IF(offspring fitness better than i)
improvement+1
ADD offspring into pop
ENDDO
IF converged on F_{β}
Evaluate pop based on F
ELSE
Evaluate pop based on F_{β}
IF (generation $\%20 = 0$)
DO
IF not converged on F_{β}
Set B based on $M(\beta)$
Evaluate pop based on F_{β}
IF improvement/population size > 0.2
Set mutation rate = mutation rate*1.2
ELSE
Set mutation rate = mutation rate $*0.8$
ENDDO
Truncate pop
ENDDO
Return best solution of pop

Fig 4. Pseudocode of EA+S

EXPERIMENTAL SETTING

For the purpose of comparison, we implemented the metaheuristic and smoothing in Evolutionary Algorithm with 20% adaptive mutation rule, called EA+S. this algorithm is compared with Classic Evolutionary Programming (CEP), Fast Evolutionary Programming (FEP), and Evolutionary Algorithm with 20% adaptive mutation rule (EA). For simplicity, selection method implemented in these algorithms is truncation. EA+S revise the β value every twenty generations. For EA and EA+S, the adaptive mutation rate is also revised every twenty generations. There are totally ten benchmark functions tested with these experiments settings. Table 1 outlines all benchmark functions. F₁ to F₉ are taken from (Xin et al. 1999) while F₁₀ is originally from (Yang and Flockton 1995).

To minimize the bias toward different type of problems between EA and EP, instead of using uniform selection for parents, each parent in EA produces exactly one offspring, as suggested in CEP and FEP (Xin et al. 1999). The only difference between EA and EP in this case is the adaptive mutation mechanism. For EA+S, the searching process is divided into two phases. In the first phase, solutions in population are evaluated with approximated function F_{β} . After the population has converged on F_{β} , the algorithm then continues the searching with the original function F.

Test Function	n	S	f_{min}
$f_1(x) = \sum_{i=1}^{n} x_i^2$	30	[-100,100] ⁿ	0
$f_2(x) = \max_i \{ x_i , 1 \le i \le n \}$	30	[-100,100] ⁿ	0
$f_3(x) = \sum_{i=1}^{n-1} [100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2]$	30	[-30,30] ⁿ	0
$f_4(x) = \sum_{i=1}^{n} -x_i \sin(\sqrt{ x_i })$	30	[-500, 500] ⁿ	-12569.5
$f_5(x) = 4x_1^2 - 2.1x_1^4 + \frac{1}{3}x_1^6 + x_1x_2 - 4x_2^2 + 4x_2^4$	2	[-5, 5] ⁿ	-1.0316285
$f_6(x) = -20 \exp(-0.2 \sqrt{\frac{1}{n} \sum_{i=1}^n x_i^2}) - \exp(\frac{1}{n} \sum_{i=1}^n \cos 2\pi x_i)$	30	[-32,32] ⁿ	0
+20+e			
$f_7(x) = \frac{1}{4000} \sum_{i=1}^n x_i^2 - \prod_{i=1}^n \cos(\frac{x_i}{\sqrt{i}}) + 1$	30	$[-600,600]^n$	0
$f_8(x) = \sum_{i=1}^{n-1} \left(x_i + 0.5 \right)^2$	30	[-100,100] ⁿ	0
$f_9(x) = a(x_2 - bx_1^2 + cx_1 - d)^2 + e(1 - f)\cos(x_1) + e$	2	$[0,15]^2$	0.397887
$a = 1, b = \frac{5}{4\pi^2}, c = \frac{5}{\pi}, d = 6, e = 10, f = \frac{1}{8\pi}$			
$f_{10}(x) = n + \sum_{i=1}^{n} x_i^2 - \cos(2\pi x_i)$	30	[-5.12, 5.12] ⁿ	0

Table 1: The Following Ten Benchmark Functions Have Been Used in Evaluating Effect of Smoothing. N Indicate The Number Of Dimension Of The Problem, S and F_{min} Indicates Function Range and Function Minimum respectively.

This is to avoid the situation where the approximated function shifted the global optimum as shown in Fig 1 and 3. For (5), the number of samples used here is the same as suggested in (Yang and Flockton 1995), which

is 10. The sample size for (10) and (12) are 500 for both. As the sample size increases, (5), (10) and (12) becomes more accurate. Further investigation of the minimum sample size is required in the future. The population size for all algorithms is set to 100, while the initial mutation rate is set to 3.0. The Gaussian random is time seeded. To avoid having different random sequence between algorithms, random sequence for (5), (10), and (12) are separated from mutation. Twenty individual runs for each algorithm is tested with all benchmark problem in table 1.

RESULT AND DISCUSSION

Recall that the purpose of smoothing in optimisation is to "pull" the population into the "area of interest" where the local optima do not exist. The ideal population that converged on approximated function should always within the "area of interest". However, the results suggested that it may not be this case. For EA+S, chances of "pulling" into the area are relatively high for F_1 , F_3 , F_5 , F_6 , F_8 and F_{10} . Consider figure 5, 6, and 7, majority of the individual runs successfully reach the area of interest, and converged on the global optimum in the second phase. EA+S suggested a huge improvement over these functions compared to EA. The reason we choose to compare our algorithm with CEP and FEP because both of these algorithms are the state-of-the-art in Evolutionary Computation. As we compare the result in table 2, EA+S always have the better quality of solution than EA, as well as FEP. The only exceptional cases are F2 and F4. Function F2 is neither polynomial nor trigonometry, which is very hard for Gaussian to estimate the pattern of the function, whereas F₄ has very sharp local optima, which requires higher β value. In fact, as shown in figure 8, function F_4 requires at lest $\beta=80$ for the approximation to be smooth. Since the maximum setting for β is 3.0 in our experiment, we expect that EA+S perform worst compare to FEP and CEP. This raises another issue where the β range has to be predetermined before the searching process actually starts. Pre-processing such as performing random walk in β space is required.

As for the comparison of the convergence speed, figure 9 and 10 shows the significant difference between the convergence speeds for EA+S and FEP for function F_8 . That is, all individual runs converged to global optimum within 500 generations for EA+S whereas only one individual run converged within 700 generations for FEP. However, this may due to several factors other than choosing the correct smoothness to approximate the function. Recall that the adaptive mutation rate for EA and EP are different. EA uses single mutation rate for all dimensions of the problem, whereas in EP, each dimension of the problem has their own adaptive mutation rate.

CONCLUSION AND FUTURE WORK

Based on the empirical results of the benchmark functions in table 2 and 3, we concluded that the metaheuristic does assist in the choosing the correct smoothness, providing a compartible underlying EA. However, its compartibility with other parameters in EA is still an open question. Further studies are required in order to understand the behaviour of Gaussian approximation in EA. We will analyse different adaptive mutation mechanism to maintain the population diversity without decreasing the probability of getting into the "area of interest". Throughout statistical learning, we may discover more meaningful information regarding the underlying problem and propose different meta-heuristic that is capable of handling various problems in the future.

	EA		Cl	CEP		FEP		EA+S	
	Mean Best	STDEV	Mean	STDEV	Mean	STDEV	Mean	STDEV	
			Best		Best		Best		
F_1	104.05	14.33	1.57	3.73	0.31	1.14	2.30E-19	5.3E-19	
F_2	3.91	0.26	12.59	5.77	7.84	4.67	6.59	6.91	
F ₃	8.89E+06	1228655	18913.85	16422.29	13347.76	20508.87	2201.243	4703.648	
F_4	-7269.24	664.2538	-7503.03	593.4426	-10587.7	412.3559	-7374.01	605.8585	
F ₅	-1.03147	0.000171	-1.03163	4.56E-16	-1.03163	4.56E-16	-1.03163	4.56E-16	
F ₆	7.936829	0.273333	8.236878	2.199107	2.271381	1.688895	4.65E-11	7.3864E-	
								11	
F_7	0.327072	0.060595	0.23566	0.153455	0.168185	0.083916	0.01958	0.010644	
F ₈	105.7	10.87779	922.3	917.0538	32.35	40.7008	0	0	
F ₉	0.397976	8.45E-05	0.397887	1.14E-16	0.397887	1.14E-16	0.397887	1.14E-16	
F ₁₀	122.505	8.64936	27.78619	8.814827	3.384301	1.814504	0.665995	0.625033	

 Table 2: Comparison Between Es and Es+S. The Mean Best and Standard Deviation Values Have Been Averaged Over

 20 Runs. Termination Condition is 3500 Generations. *Stdev is Abbreviation of Standard Deviation.

*Mean Best with **BOLD** indicates that there are 95% confindence that they are statistically significant different compare to EA+S in T-Test. Mean Best with *Italic* in EA+S column indicates it is the best among others.



Fig 5. Natural Log Of Best Fitness of 20 Individual Runs of EA+S In 3500 Generations for Function F_1 .



Fig 6. Natural Log Of Best Fitness of 20 Individual Runs of EA+S In 3500 Generations for Function F₃.



Fig 7. Natural Log of Best Fitness of 20 Individual Runs of EA+S In 3500 Generations for Function F_{10} .



Fig 8. Single Dimension of Function F₄ With y-axis as The Fitness Value Against x-axis, and Beta=50, 80.



Fig 9. Natural Log of Best Fitness of 20 Individual Runs of FEP In 3500 Generations for Function F₈.



Fig 10. Natural Log of Best Fitness of 20 Individual Runs of EA+S In 3500 Generations for Function F₈.

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MODELLING THE RESPONSE OF BAMBARA GROUNDNUT: A KEY UNDERUTILISED CROP IN AGRICULTURAL SYSTEMS

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KEYWORDS

Bambara groundnut, BAMGRO model, AquaCrop model, abiotic stress, landrace

ABSTRACT

Bambara groundnut (Vigna subterranea (L.) Verdc) is an indigenous legume that is still cultivated in subsistence agricultural systems in sub-Saharan Africa, despite any major research effort until recently. The crop is cultivated from local landraces as until now there are no true varieties of the species bred for specific traits. The variable and hostile climates in the region mean that annual yields of most rainfed crops including bambara groundnut are far below their agronomic or genetic potential. The lack of quantitative information on the eco-physiological responses of the crop to various abiotic factors has resulted in poor decision making on crop management practices especially in relation to sowing date and the selection of appropriate landraces for different locations. The present modelling approaches via BAMGRO and AquaCrop models provide useful predictive information on canopy development, biomass production and yield formation of bambara groundnut landraces under contrasting environments. Two contrasting landraces; Uniswa Red (Swaziland) and S19-3 (Namibia) were used in the present study to evaluate the growth and yield performances under drought, heat and cold stress.

The comparison of model simulations with experimentally observed values demonstrate that canopy development, biomass production and yield are statistically acceptable with a high correlation $(r^2; 1:1)$ with line of identity and lower RMSE. Recent approaches of calibration in FAO-AquaCrop reported that the observed CC%, biomass and end of season yield under glasshouse (Nottingham, UK) and field (Africa) can be well explained in model simulations. Further, the extension of the present dynamic model BAMGRO for inclusion of landrace parameters based on molecular genetic estimates is introduced as a novel approach in modelling bambara groundnut. A model that links physiological/trait data and/or molecular genetic estimates of genetic width of a landrace will provide the potential for further improvement of this underutilised species. Further, our multidisciplinary experience with one underutilised crop i.e. bambara groundnut integrated into a global system i.e. AquaCrop can act as a generic basis to model many other underutilised species that can play an important role in the agricultural systems of the future.

INTRODUCTION

The agricultural systems in semi-arid regions of sub-Saharan Africa are normally characterised by extreme climatic conditions. Some of the most resilient crop species such as sorghum (*Sorghum bicolor*. L. Moench), pearl millet (*Pennisetum Americanum*) and cowpea (*Vigna unguiculata*). have originated from this region. Globalization challenges the existence of these indigenous crops with less resilient, but more popular crops like maize (*Zea mays*) and bean (*Vicia faba*), which are higher yielding under favourable climates. In addition, the improved breeding programmes of major crops have widened the gap between the cosmopolitan and traditional crops.

Bambara groundnut (*Vigna subterranea* (L.) Verdc) is one such indigenous legume with significance as a source of protein in sub-Saharan Africa where it is mainly grown by women farmers for the subsistence of their families. Its nutritional composition (protein content is 16-25%) is highly comparable or superior to other legumes (Linnemann and Azam-Ali 1993), providing an important supplement to cereal-based diets. In the absence of established varieties, marginal and subsistence farmers in Africa grow locally selected 'landraces' of bambara groundnut. A landrace is a locally adapted strain of a species selected through traditional methods and not influenced by modern breeding technologies.

The production and consumption of bambara groundnut is mainly confined to semi-arid Africa where very low and erratic distribution of rainfall, losses through runoff, drainage and evaporation result in limited available

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soil moisture for crop growth. According to Azam-Ali and Squire (2002), the agro-ecological niche of bambara groundnut is similar to that of millet and groundnut based on the observations that it appears to be more tolerant of drought conditions than other legumes (Linnemann and Azam-Ali 1993). In spite of the drought tolerant capabilities of bambara groundnut, results reported by Collinson et al. (1996) suggested that canopy expansion, biomass production and yield are reduced under strong drought stress.

Temperature variability is a yield determining factor in many parts of the world including semi-arid Africa where bambara groundnut is normally grown. The wide fluctuations in daily mean temperature in semi-arid Africa necessitate a thorough understanding of the effects of heat and cold stress which may both affect growth and development in the same season. Extremes of temperatures are a major constraint to crop adaptation and productivity; especially when they coincide with drought and critical growth stages of plant development.

To explore the potential growth and yield of bambara groundnut landraces in various agro-ecological regions and to evaluate the possibilities of transferring them to a different locations, it is vital to understand how crop processes are influenced by major environmental factors. The numerous permutations of abiotic factors that may affect growth and development mean that research has prioritised the quantification of key environmental factors through the use of suitable modelling approaches.

The heuristic value of a crop model for determining growth and yield are well established (Sinclair and Seligman, 1996). The broader goal of a crop model is to simulate and explain crop development, growth and yield as functions of environment, management and genetically controlled characteristics.

In this paper, the response of bambara groundnut is presented through the use of a new crop model (BAMGRO) integrated into the UN-Food and Agriculture Organisation (FAO) AquaCrop model (http://www.fao.org/nr/water/AquaCrop.html).

BAMGRO is based on the established CROPGRO model (Boote et al. 2002a) and collectively both BAMGRO and AquaCrop simulate responses to abiotic stress with special reference to drought, heat and cold. Subsequently approaches for linking molecular information within BAMGRO/AquaCrop are outlined.

A crop simulation model for an agronomically and nutritionally variable crop like bambara groundnut will provide the framework for scientific cooperation to rapidly integrate new knowledge and prioritise future research on an under-researched and underutilised species. This new approach to model bambara groundnut responses to major abiotic stress factors provides a platform for easily incorporating other biotic and abiotic factors and extending the model to more landraces and ultimately varieties of the crop. These modelling approaches linked with integrated research have useful lessons for the modelling of other underutilised crops and their potential for future agricultural systems.

MODEL DATA SETS

Briefly, datasets from glasshouse experiments in Sutton Bonington Campus, University of Nottingham, UK (Tropical Crops Research Unit; TCRU) in 2002 and 2006 were used to calibrate BAMGRO. The FAO-AquaCrop model was calibrated for bambara groundnut using all the data sets from glasshouse, UK (2002, 2006, 2007, 2008) and field observations in Swaziland to represent different growing conditions.

The details of experimental design, plant sampling procedures, irrigation treatments and standard measurements for TCRU-2002 experiment have been previously explained in Mwale et al., (2007a). BAMGRO was validated using independent datasets from 2 years of Glasshouse experiments, Nottingham, UK (TCRU-2007, TCRU-2008) and field experiments in Swaziland.

Over the summer months of 2006, 2007 and 2008 (April to September), two contrasting bambara groundnut landraces; Uniswa Red (Swaziland) and S19-3 (Namibia) were grown in five glasshouses with each house having one Uniswa Red and one S19-3 plot under controlled temperature regimes. Two temperatures 23±5 ${}^{0}C$ (LT) and 33±5 ${}^{0}C$ (HT) were imposed in the five glasshouses. Soil moisture in each house was nonlimiting with weekly irrigation to field capacity until harvesting in 2006, up to 77 DAS in 2007 and up to 33 DAS in 2008. The treatments were allocated according to a split-plot design that combined two bambara groundnut landraces (Uniswa Red, S19-3) and two different temperature regimes (LT, HT) with each treatment replicated twice and thrice at low and high temperature, respectively, due to limited number of glasshouses.

As described by Cornelissen (2005), from December 2002 to May 2003 a set of Swaziland and Botswana landraces were grown in field sites in Swaziland (Malkerns and Luve) and Uniswa Red was selected for the present validation of BAMGRO as it is common to the landraces grown in glasshouse conditions at Nottingham, UK. During the experimental period Malkerns reported well distributed rainfall thus suggesting no water limitation while the crop experienced a severe drought stress in the Luve field site.

MODEL DESCRIPTION

Summarised details of BAMGRO and AquaCrop models are described below.

BAMGRO Model

BAMGRO is intended to predict the performance of different landraces under variable climates. Bambara groundnut is an indeterminate crop so leaf production can occur from emergence until maturity, depending on the supply of assimilates available and the effects of stress due to drought and temperature. Also, a fraction of produced leaves is removed from the plants as dead leaves due to senescence. Therefore, the rate of daily increment in actual leaf number (*LN*) can be explained as the balance between rate of new leaf production (LN_{new}) and rate of leaf senescence (LN_{dead}) as in Equation (1).

$$\frac{dLN}{dt} = LN_{new} - LN_{dead} \tag{1}$$

Thereby the leaf area expansion (LA) is calculated as a function of rate of leaf production and landrace coefficient *a* according to Equation (2).

$$LA = a \times LN \tag{2}$$

Actual increase in dry matter (DM_{actual}) is calculated from the minimum of two potential growth rates (Equation (3)), one determined by intercepted radiation (Light Limited Growth-*LLG*, Equation (4)) and the other by soil water supply (Water Limited Growth-*WLG*, Equation (5)).

$$DM_{actual} = \min(LLG, WLG)$$
 (3)

$$LLG = PAR \times S_i \times \varepsilon_s \times (1 - \exp^{-k \times LAI})$$
(4)

$$WLG = \frac{\left(U_{soil} \times TE\right)}{SD}$$
(5)

Where, S_i is short wave solar radiation (MJ day⁻¹ m⁻²), *PAR* is Photosynthetically Active Radiation (50% of S_i) ε_s is efficiency of conversion of this solar radiation (g MJ⁻¹), *LAI* is leaf area index, *k* is light extinction coefficient, U_{soil} is potential rate of water uptake by roots in profile (mm d⁻¹), *TE* is transpiration efficiency (g mm⁻¹) and *SD* is, saturation deficit (k Pa).

Dry matter (DM_{actual}) partitioning gives priority to above ground parts (leaves and stems) during vegetative growth and towards pods during reproductive phase. At the end of each simulated day, remaining biomass is directed towards roots based on the requirement of the roots that is adjusted according to growth phase and stress condition. Pod formation (*PN*) and pod filling (*PW*) are considered as two independent processes during the reproductive phase and contribute towards the pod yield.

To model the effect of soil moisture stress (*WSTRESS*) on growth and development, a relationship *WLG* (Equation (5)) and *LLG* (Equation (4)) is considered. The value varies from zero to one where one represents no stress and zero represents maximum stress.

When the crop is exposed to a range of temperatures within the boundary line of base (T_{base}) and ceiling (T_{high}) temperatures, it results in potential temperature stress and the stress index (*TSTRESS*) ranges between zero and one like in *WSTRESS*.

AquaCrop Model

AquaCrop is a water-driven crop-model aiming at simulating yield response to water of herbaceous crops. AquaCrop describes crop foliage development in terms of canopy cover (*CC*, Figure 1) and not via *LAI*. This distinctive feature introduces a significant simplification, allowing the user to enter actual values of CC even estimated by eye.



Figure 1: Green canopy cover development described by four parameters: initial canopy cover at the time of crop emergence (CCo), canopy growth coefficient (CGC), expected maximum canopy cover (CCx), canopy decline coefficient (CDC)

Canopy cover is used for the computation of transpiration. Using Water Productivity (*WP*), AquaCrop calculates above-ground biomass production from transpiration (Tr) and reference evapotranspiration (*ETo*) (Equation (6)).

$$m_i = WP \times \frac{Tr_i}{ETo_i}$$
(6)

Where, m_i is the daily above-ground biomass production, Tr_i is the daily crop transpiration, ETo_i is the

daily reference evapotranspiration, and WP* is the normalized water productivity.

The model is based on the conservative behavior of WP (de Wit 1958, Hsiao and Bradford, 1983, Steduto et al. 2007), that is the constancy to the relationship between biomass production and transpiration. The normalization of WP for climate (atmospheric evaporative demand, ET_o , and concentration of the bulk atmosphere, CO₂) makes AquaCrop applicable to diverse location and seasons, including future climate scenarios.

AquaCrop does not calculate the partitioning of biomass to various organs, but simply adopts the Harvest Index (*HI*) to simulate the portion of above-ground biomass stored into the grains (yield). This choice avoids dealing with the complexity and uncertainties associated with the partitioning processes.

AquaCrop simulates water stress in terms of its effects on leaf growth, stomata conductance, canopy senescence, and *HI*. With the exception of *HI*, these effects are manifested through individual stress coefficients (K_s). K_s varies from one (no stress) to zero (the stress effect is maximum), and it is function of water content in the root zone.

Temperature plays a role in influencing crop development, when the Growing Degree Days (*GDD*) mode is chosen. Biomass production might be hampered when the air temperature is too cool, through a temperature stress coefficient (K_s). In addition, cold or heat stress at flowering might induce a reduction in *HI*.

Proposed Genetic Linkage Model

A new approach has been initiated within the BAMLINK project (Sean Mayes), University of Nottingham, UK (Mathematics in Plant Sciences Study Group http://cpib.info/study2008/programme.shtml) to link existing genetic marker and physiological data as a test case using the BAMGRO/AquaCropmodel to evaluate the effect of genetic variability *per se* on physiological traits. It will provide information on how much intra-landrace genetic viability contributes to each trait, or to 'traits' more generally.

Large marker datasets are currently in development It is likely that intra-landrace genetic variability will actually be a variable in the model that is built, in the first instance. This model would be able to derive results which estimate the required amount of genetic 'width' data to optimally inform the physiological data, for a number of scenarios. A partial validation will be carried out with existing (limited) data.

In order to assess model performances and provide an objective evaluation of the "closeness" of simulated (S) vs. measured (M) values, a number of indicators are used. Visual observations provide comparisons for

either over or under estimations. Coefficient of determination with 1:1 line is the conventional r^2 statistic, applied to the line of identity (r^2 ; 1:1) (Equation (7).

$$r^{2} = \left(\frac{\sum \left(M_{i} - \overline{M}\right)^{2} - \sum \left(M_{i} - S_{i}\right)}{\sum \left(M_{i} - \overline{M}\right)^{2}}\right)$$
(7)

SIMULATION RESULTS

BAMGRO Model

The model comparison for pooled data from glasshouse experiments, Nottingham and field experiments in Swaziland on *LAI*, Total Dry Matter (*TDM*) and yield (Y) over the season for each landrace correlated well with measured values. The statistical evaluation of the model reported that *LAI* is well correlated with the line of identity indicating acceptable correlation coefficients (r^2 ; 1:1 line) for S19-3 (0.83) and Uniswa Red (0.78). Similarly, yield simulation of BAMGRO was statistically acceptable with higher correlations (r^2 ; 1:1 line for S19-3 (0.87) and Uniswa Red (0.61)) and less than 0.5 t ha⁻¹ of RMSE value.

AquaCrop Model.

The linear regression of simulated vs. measured canopy cover (*CC*) shows an over- and under estimation of not more than 3%, which is much less than the degree of error in measuring the data at field level. Further, the slope of the regression line (0.91) and the intercept (2.97) are not significantly different to the slope (1.0) and the intercept (0) of 1:1 line. The canopy cover formation is explained successfully by AquaCrop model indicating high r^2 (0.88). RMSE (15%) was acceptable, considering the degree of error in the data at field level in Africa and the Glasshouse in Nottingham, UK due to the differences in solar radiation intensities.

The linear regression of simulated vs. measured biomass shows a very small over-estimation at the early stage. However the slope of the regression line (0.95) and the intercept (0.23) are not significantly different to the slope (1.0) and the intercept (0) of 1:1 line. Biomass production is explained successfully by AquaCrop indicating high r^2 (0.78). RMSE (0.78 t/ha) was acceptable

Simulation of end of season yield can be considered satisfactory with relatively higher R^2 (0.72), with RMSE (0.36 t/ha) lower than half ton/ha (data not shown). AquaCrop version 2.9 was used for the present calibration and version 3.0 provides more mechanistic approaches to overcome the problems associated with yield simulation in version 2.9. Therefore better results can be obtained by most recent version 3.0.



Figure 2. Comparison between measured and simulated *LAI* for Uniswa red and S19-3 in glasshouse experiments, Nottingham, UK and field sites in Swaziland. Model data sets were provided by Ibraheem Alshareef, Stanley Noah and R.Cornelissen.



Figure 3. Comparison between measured and simulated pod yield for Uniswa red and S19-3 in Glasshouse experiments, Nottingham, UK and field sites in Swaziland. Model data sets were provided by Ibraheem Alshareef, Stanley Noah and R.Cornelissen.



Figure 4. Model calibration results of AquaCrop model for canopy cover (*CC* %) and biomass for four landraces (Uniswa Red, S19-3, DipC and OM1) in glasshouse experiments, Nottingham, UK and field sites in Africa. Model data sets were provided by Ibraheem Alshareef, Stanley Noah, R.Cornelissen (University of Nottingham.

DISCUSSION

The validation of the BAMGRO and calibration of the AquaCrop models show some deviations of model prediction for two different growth conditions (glasshouse and field) under drought, heat and cold stress. Therefore the possible reasons for these discrepancies may be the landrace variability ('genetic width' the differences in quality and quantity of solar radiation during UK summer and in semi-arid Africa and model structure.

CONCLUSIONS AND FUTURE WORK

BAMGRO model validation results for canopy development and yield for the tested two landraces (Uniswa Red and S19-3) are in good agreement with measured values in glasshouse conditions in Nottingham, UK and field sites in Swaziland. However, Uniswa Red reported wider distribution of simulations consistently in *LAI* and yield compared to the Namibian landrace, S19-3 thus providing opportunity for extending the model to genetics.

Bambara groundnut was successfully included in the FAO-AquaCrop phase providing evidence for possibility of inclusion of other underutilised crops in this interface.

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SPACE-PARTITION BASED IDENTIFICATION OF PROTEIN DOCKSITES

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KEYWORDS

Protein Docksites / Information Granules, Space-Partitioning, Multi-Resolution Modelling

ABSTRACT

A new method for identifying protein docksites is presented here. We introduce a space-partition based technique for evaluating the binding areas of a protein and present the final output in a 3-dimensional environment. The experimental space is tessellated through bi-partitions and the occupancy of each atom within the tessellations is approximated using evaluated constraints. A series of preprocessing steps are taken to ensure that the subject of experiment is independent of orientations and thus gives reproducible results. The final modelling of the protein shows the docksites granulated using a compactness criterion. Controls of the compactness limit the clusters of binding sites to be displayed on the 3D projections with more prominent areas linked to a higher compactness of 3D structures.

INTRODUCTION

With the increasing number of proteins being added into the Protein Data Bank (PDB) there is a need for fast and efficient algorithms to process these files and derive important information for further analysis. Each protein – formed from a series of amino acids – may fold to reveal a completely different structured protein although the base chain may be similar. The binding sites of a protein are the areas that contribute to the protein's functions. Hence it is important to identify these docksites and conduct analysis upon them to gain a better understanding of the protein.

There are many methods available today for the identification of protein docksites. For example, POCKET - developed by Levitt and Banaszak [Levitt, Banaszak, 1992], is able to identify the docksites of a protein through the use of cubic grids without the need for prior knowledge of proteins. However. disorientations in the protein will lead to a reduced efficiency of the algorithm. LIGSITE [Hendlich et al., 1997] remedied the weaknesses of POCKET by using rigorous scans. SURFNET, created by Laskowski [Laskowski, 1995], visualises molecular surfaces and the gaps in between which indicate potential cavities.

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors) ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD) The program is interactive and is compatible with other graphics packages. Although each algorithm has its own strong points, none of the current solutions is fully satisfactory. Research is still continuously being conducted to find better solutions [Ritchie, 2008].

Here we present a new way of looking at the problem of identifying protein docksites. The notion of spacepartitioning is introduced here. Our technique attempts to recursively 'slice' a fixed experimental space into smaller and smaller subunits until the minimum threshold is achieved. The protein is then cast into the experimental space and a checking is made to verify if a particular voxel is occupied by any of the protein's atoms. We do not use exact measurements but rather a way of generalising the data, which greatly increases the processing speed but also maintains the vital information required.

The final modelling of the predicted docksites of the protein is carried out on a multi-resolution basis. Information granules contribute to and determine how the modelling algorithm runs. By using the same set of original data, a series of processing is carried out to extract and compose a range of data which can be studied on different levels. The information granules gathered may be clustered together such that a more generalised representation is obtained. Alternatively, the granules may also be broken down for more refined data analysis. Multi-resolution modelling is a visualisation of these granules and hence, our modelling program displays the detected docksites of a protein in terms of coarse and detailed representations.

BACKGROUND

It can be seen from previous research that cubic grids offer an efficient means for protein analysis. Such grids also form the underlying structures for our spacepartitioning algorithm. In space-partitioning, a given experimental space is tessellated into subunits of smaller spaces, whereby the size of the subunits are dependent on the type of partitioning algorithm employed. For this research, the bi-partitioning method is used. This technique is fast and executes in $\log_2(n)$ time. For example, a test space of size 80 will be subdivided into units of size 40, followed by units of size 20 and so on. The algorithm stops when the minimum threshold has been reached.

Bi-partitioning may seem similar to the concept of fractals but it should be noted that there are noticeable differences in both. The partitioning of a space has constraints applied to it and the end result should be somewhat balanced. It is a recursive process similar to the generation of fractals but unlike the latter it generates regular shapes, which in this case are hyperboxes. Therefore, one can say that spacepartitioning has a fixed scale applied to ensure that the subdivisions are always consistent.

We can say that information displays the attributes of fractals – one can granulate the data and analyse the output on different stages in terms of fuzzy modelling [Pedrycz, Bargiela, 2003]. Wang et al [Wang et al, 1990] did a study and identified the relationship between fractal dimensions and the tertiary structure of proteins, proving that such an approach is applicable within this domain. Hu and Peng [Hu, Peng, 2005] developed a measurement termed Volume Fractal Dimensionlity (VFD) which may be employed in the study of protein evolution and prediction.

Our approach to identify the docksites on a protein attempts to process an original PDB file - obtained from RCSB Protein Data Bank (http://www.rcsb.org) in several stages. A PDB file contains all vital information related to the protein, including the spatial coordinates of each atom, the atom type, the occupancy of each atom etc. However only 4 items of data are required in the algorithm – the X, Y, Z coordinates as well as the Van der Waals radius for each of the atom. The VDW radius gives an estimation of the size of the entire atom, which corresponds well to our objective of approximated analysis and modelling. By using the above data, we first preprocess the protein so that it is invariant to translation and rotation. It should be noted that a change in the orientation of the protein has posed problems for researchers over the years. We hereby introduce a novel method of aligning the protein to overcome all disorientations. Further details are elaborated in the Preprocessing Section.

The new set of preprocessed data is then sent for the generation of 2-dimensional templates whereby the space-partitioning algorithm is duly applied. We choose to partition in 2D instead of 3D as the additional dimension will increase the computation and memory usage significantly. To overcome the problem of the missing dimension, we selected the dimension not portrayed in 2D for unit slicing. By unit slicing we mean that the dimension concerned will be split based

on the smallest unit used. This is similar to z-buffer algorithm in 3D graphics. A list of images are then generated using the other two dimensions. The number of images is related to the count of segments obtained from the sliced dimension. More elaboration is given in the Space-Partitioning Section.

The final stage of the program involves projecting the processed data into the 3-dimensional space. The Java 3D package is harnessed here and the 2 smallest partition levels are included in the program for visualising the concept of multi-resolution modelling. Each partition level is given a set of controls whereby the occurrences of higher or lower weighted docksites can be manipulated by changing the values. A more detailed description is presented in the section on modelling.

PREPROCESSING

The objective of the preprocessing stage is to ensure that the chosen protein is aligned with the axes in the experimental space. This method is an attempt to overcome the problem of disorientations encountered in previous research works. The algorithm has been tested for the same protein rotated in all X, Y and Z planes and has proved to be effective in realigning the protein consistently.

The first step in the preprocessing stage is the calculation of the maximum-valued cross sectional cord between all atoms in the protein. The calculation is carried out in 3D space whereby the equation is given by Equation (1).

$$D = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}$$
(1)



Max Cross Section Distance

Figure 1: Illustration of the Maximum-Valued Cross Sectional Cord

Once this value has been obtained, the algorithm proceeds to align the cord such that it is parallel with the X axis in 3D space. The maximum cord always gives the same value regardless of how the protein was initially positioned. Affine transformations are used here and the matrices are given in the equations below.

$$T = \begin{bmatrix} 1 & 0 & 0 & dx_i \\ 0 & 1 & 0 & dy_i \\ 0 & 0 & 1 & dz_i \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad T^{-1} = \begin{bmatrix} 1 & 0 & 0 & -dx_i \\ 0 & 1 & 0 & -dy_i \\ 0 & 0 & 1 & -dz_i \\ 0 & 0 & 0 & 1 \end{bmatrix}$$
(2)

$$Rz = \begin{bmatrix} \cos\varphi & -\sin\varphi & 0 & 0\\ \sin\varphi & \cos\varphi & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1 \end{bmatrix}$$
(3)

$$Ry = \begin{bmatrix} \cos\theta & 0 & \sin\theta & 0\\ 0 & 1 & 0 & 0\\ -\sin\theta & 0 & \cos\theta & 0\\ 0 & 0 & 0 & 1 \end{bmatrix}$$
(4)

In affine transformation all the spatial coordinates of the object are first translated with relation to the origin. Subsequently rotations around the z and y-axis are carried out. The final step involves moving the object back into the original space. Equation (2) gives matrices for translation to the origin and back to experimental space. In the program, one of the points of the maximum cord is selected as the point of reference for translation to origin. All atoms are translated with relation to this point. Following that the protein is first rotated about the Z-axis followed by a rotation about the Y-axis. Equations (3) and (4) are the corresponding transformations. The angles for each of the matrices are illustrated in Figure 2.



Figure 2: Angles of Rotation Around Y-axis and Z-axis

Applying the above rotations will ensure that the maximum cord gets aligned with the X axis, resulting in a value of 0 for both Y and Z axes for all points on the cord. However this does not solve the protein missalignment completely. The protein may need to be rotated around the X axis to a position that ensures reproducible positioning of the protein.

$$Rx = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha & 0 \\ 0 & \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$
(5)



Figure 3: Results of PDB300d after Preprocessing. Originals (clockwise from top left) are rotated 60° about Z, 120° about Z, 10° about X, 20° about Y, 30° about Z and 30° about Y, Z.

Our approach is to identify an atom that is furthest away from the cord and to align the orthogonal projection from this point onto the cord with the Y axis. The matrix representation for rotation about X axis is given in Equation (5). Therefore, the complete affine transformation of the protein involves translation to the origin, carrying out the rotations about all the axes, and translating the protein back into the experimental space by a fixed amount. This preprocessing has been tried on different inputs and the results show consistency regardless of the initial positioning of the protein. Figure 3 shows a few of the output generated in 2D.

SPACE-PARTITIONING

The preprocessed datasets are sent for the generation of 2-dimensional templates in the form of images. As mentioned in Background, one of the dimensions is selected for unit slicing, which in this case is the Z dimension. Take for example the protein that has atoms occupying units 300 to 900 in Z dimension and the smallest unit space used is 10 units. Unit slicing will proceed to generate an analysis image for every 10-unit interval within the occupied range. The output images are then generated using the other 2 dimensions following space-partitioning. The images in Figure 4 show output of different layers after bi-partitioning has been applied.

Notice that the images contain different shades of boxes. These boxes are generated from the bipartitioning algorithm. The darker gray shades on the left of the images are obtained from the first run of bipartitioning. As no part of the protein occupy these spaces, hence they are shaded.





The bi-partitioning algorithm starts from the whole of the experimental space and continues executing until the smallest unit is reached. The smallest unit is chosen based on an analysis of the sizes of atoms in proteins. There is no merit in subdividing the units beyond this size as this would increase the processing and decrease the efficiency of the algorithm without adding any significant information about the topology of the binding sites. The objective is to keep the voxels sizes just small enough such that information on the protein is not lost. Generating the voxels on a subatomic basis does not necessarily increase the details needed. Such space-partitioning method looks at the predictions of the docksites on a multi-resolution level. The first few runs executed at coarse resolution generally do not tell the user where the docksites are, but they do limit the experiment space to where the protein resides. Further runs of the algorithm with increasing resolution begin to indicate to the user the potential docksites and the final run with the highest resolution gives a clear definition of the binding areas by lining the edges of the docksites with boxes of the smallest unit.

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	1
2	2	1
1	l	1

Figure 5: How The Bi-Partitioning Algorithm Works

Figure 5 shows how the bi-partitioning algorithm works. The numbers in the grids correspond to the runs, i.e. 1 is Run 1, 2 for Run 2 and so on.

There are some techniques of image processing employed here to increase the speed of the spacepartitioning algorithm. First of all an imprinting of the protein is created on a temporary image in a solid colour. Then the pixels of a partitioned space from the temporary image are checked to see if it is being occupied by any atom. If it is empty, then the partition is given a colour or shade on another new image.

PartitionSize = The Test Space Dimension
FOR 0 to Test Space Dimension
FOR each PartitionSize
Check if partition contains atom
IF YES
Leave partition unshaded
ELSE
Shade partition based on
current partition color
END OF CHECK
END FOR
Decrease PartitionSize by half
END FOR

Figure 6: Pseudocode for the Bi-Partitioning Algorithm

If however, an atom partially occupies a partition, then a constraint is applied to decide if the protein should be given the partition or if the partial occupancy should be excluded. This is a method of estimation which maintains the necessary information while discarding insignificant ones.

The checking for the images is carried out for each and every slice and the unit information for two of the smallest partitions are exported to files for use in modelling. By using comparison between images, the amount of time used is decreased as the process involves only simple comparisons between pixels. The bi-partitioning algorithm is given in pseudocode in Figure 6.

MODELLING THE IDENTIFIED PROTEIN DOCKSITES

After the space-partitioning algorithm has been applied to every image generated, there is a list of datasets available for visualisation in the 3-dimensional space. Here we harness the power of the Java3D package as our modelling and visualisation tool. The program output has a universe showing groups of unit voxels which fill the potential docksites and a control panel for users to update the compactness factor. This factor characterizes individual voxels and enables control over granulation of voxels into docksites. The images below show comparisons between the output from different levels of compactness factors at the same sites. Higher compactness factor implies display of only the voxels that are highly connected between themselves and lower compactness factor permits display of less well connected voxels.



Figure 7: Voxels of Unit 10, with Compactness Factor of 60 and 55 respectively



Figure 8: Voxels of Unit 20, with Compactness Factor of 60 and 50 respectively

A method for the calculation of the connectivity of the voxels has been devised so as to enable the user to control the display of the docksites according to their compactness factor. By using the information from the datasets generated from space-partitioning, a list is constructed to store unique entries of the points of cubes existing for each partition group. At the same time, the number of times each point is used is also stored into memory. A standalone cube has each of its corners given a value of 0 as none of the points are interconnected with other cubes. The sum of the points determine the total weight for that cube, which in this case is 0, making the cube a least significant voxel. This weight is interpreted as a compactness factor of the docksite. A higher total weight indicates that the cube is highly interconnected with other cubes, suggesting that it contributes more to the group of voxels which collectively form the binding agent for a potential docksite. By allowing the user to select which compactness factor should be used for visualizing docksites, the program becomes an analysis tool for revealing potential crevices in the protein. The images below provide a clearer idea of this approach.



Figure 9: Illustration of A Single Corner On A Voxel Connected to Another Voxel



Figure 10: Illustration of A Moderately Connected Voxel with Total Weight 10

Figure 9 shows a single point connectivity between the main subject and a neighbouring voxel. The total weight for the voxel is 1. In Figure 10, the main voxel has 4 neighbouring cubes. Three of its corners are each shared with two other cubes and four corners are each shared with one cube; thus making the total weight for this cube equal 10. Such sharing does not violate the uniqueness of the points, but rather contributes to the total weight of the voxel concerned and defines the level of significance of the voxel within a cluster. The higher the total weight, the heavier the role of the voxel in a particular docksite group. The maximum sum any corner of a voxel can achieve is 7, which is a full neighbourhood connectivy, making the maximum total weight 56.

In our visualisation program, we have added controls for users to update the compactness factor of the docksites. Users are given the opportunity to increase or decrease the weight while observing how differences in the values affect the voxels in the 3-dimensional universe. As the weight value decreases, voxels with lesser neighbourhood cubes are gradually introduced. The higher the factor value, the more compact and smaller a docksite binding cluster becomes. However it should be noted that there is an optimum threshold for the clusters. Once beyond this threshold, the docksites information may tend to overcluster, leading to a less than accurate output. Likewise an overly high compactness value may also lead to underclustering. Determination of this optimum value is a study in itself and requires further analysis.

As of current, it is sufficient to show that given the flexibility to control the weights of the clusters, such a visualisation program is able to aid researchers and scientists in the investigation of potential protein docksites and in the prediction of possible docking elements through the analysis of the models of the displayed clusters.

DISCUSSION

There is much merit in the use of cubic units or voxels in identifying potential protein docksites. This could be due to its simplicity and the reduced processing time as it does not require complex mathematics. The approach proposed here is considerably fast, with the spacepartitioning stage completing in a matter of minutes on a normal workstation. Increasing the processing power of the machine will reduce the time involved in partitioning the spaces. The modelling of the voxels in 3-dimension is based on the results generated and computation for determining the voxels to be displayed is fast enough such that a change in the compactness factor updates the 3D universe in seconds.

An advantage of using cubic units in studying the surface of the protein is the ability to shortlist the corresponding units for further analysis. Methods like convex hull assignments [Stout et al, 2008] or Bezier splines do provide a mapping of the protein structure and surface to some extent, but some crevices in the protein may tend to get ignored or generalised unless richer input is supplied. Compared to these approaches, the use of cubic units and space-partitioning is able to cater for a more refined level of analysis, allowing for the extraction of particular sections. Cubic units also provide a clearer estimation of the shapes of possible binding agents.

In our approach we have overcome the problem of misalignment of the protein in the 3D space. The method is straightforward and fast, and results have shown to be promising in terms of reproducible alignment of the protein. The use of multi-resolution modelling here provides a new insight into the analysis of data from a single protein, especially in locating the docksites of a protein. Through simple controls one can choose to show or hide a particular set of information granules, allowing for different levels of studies. Coarser granules give general representations while refined ones display more information. With different resolutions one can create programs that work on different datasets – often a coarser granulation will lead to faster processing. Such approach works on the approximation plane while retaining the right amount of information for the user.

Granular modelling is emerging as a new paradigm for the classification and processing of information. By introducing this concept into the field of bioinformatics new methods can be produced whereby the use of fuzzy processing may lead to a comparable if not better achievement of results. In our research it is important to correctly identify the docksites on a protein and by utilising an outside-in approach the shapes of potential binding agents can be estimated. Granular modelling generates different levels of granularites for these predicted binding agents and the visualisation program has included 2 sets of controls for viewing the agents in different levels. For each level of granularity ranging from coarse to fine, we can obtain varying degrees of information - a course representation provides us with clues on the locations of the docksites and as the representation becomes more and more refined the shape of the binding agent becomes more well described.

CONCLUSION

The space-partitioning method provides a new and novel approach of identifying docksites in a protein. By using a newly devised algorithm, the protein file is preprocessed such that it is invariant to disorientations. The bi-partitioning algorithm is then executed on the preprocessed data, resulting in a new list of images and voxel information which is then used for the modelling of the located docksites. Controls for the compactness factor are given in the visualisation program. By updating and changing these values, users may observe an immediate update of identified docksites being projected or removed from the 3-dimensional universe. These docksites are represented on 2 levels of resolution, providing information on a rough and refined basis. The use of this multi-resolution approach not only extracts the necessary information from the data through estimation, but it also preserves the vital information needed. There are significant advantages of using a cubic grid system over more conventional methods which employ surface curves in the analysis of proteins. Cubic grids are able to locate more precisely the potential docksites and possibly provide a predicted solution to the docksite.

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HIERARCHICAL METHOD FOR NURSE ROSTERING BASED ON GRANULAR PRE-PROCESSING OF CONSTRAINTS

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ABSTRACT

Nurse Rostering problems represent a subclass of scheduling problems that are hard to solve. Their complexity is due to the large solution spaces and the many objectives and constraints that need to be fulfilled. In this study, we propose a hierarchical method of granulation of problem domain through preprocessing of constraints. A set of zero-cost patterns in the granulated search space provides a basis for the generation of work schedules. Feasible schedules calculated for week 1 are used to define zero-cost shift patterns that can be deployed in week 2. These in turn are used for the generation of feasible schedules for week 2. The process can be applied over the extended time frame. We show that the granulation of the problem description in terms of constraints and scheduling time frames leads to a more manageable computing task.

INTRODUCTION

In recent years, many hospitals have moved to selfscheduling where nurses create their own rosters based on eligibility and contractual agreements. When conflicts occur, adjustments are made through consensus. Although it is easy to implement, selfscheduling may not be practical in all situations. As a consequence, more systematic approaches have been developed (Hadi and Jonathan, 2007).

Nurse rostering is concerned with highly constrained resource allocation problem in to slots in a pattern, where the pattern denotes a set of legal shifts. In nurse rostering, the ultimate aim is to create high quality timetables, considering the well-being of nurses and the operational concerns of the employers (Ozcan 2005). Typical issues concerned with nurse rostering include coverage demand, day-off requirements, weekend-off requirements, minimum and maximum workforce, etc (Brucker et al. 2005).

A wide variety of different methodologies and models have been developed to deal with different problem circumstances during the years (Cheang et al. 2003, Ernst et al. 2004, Sitompul and Randhawa, 1990). These include mathematical programming (Beaumont, 1997, Pierskalla and Rath, 1976, Warner, 1976), meta-heuristic methods such as Genetic Algorithms (GA), Constructive Heuristic, Simulated Annealing, Tabu-Search, Multi Objective Approach (Aickelin and Dowsland, 2003, Burke et al., 2001, Burke et al., 1998, Duenas et al., 2003, Gendrau et al., 2003and constraint satisfaction techniques (Adbennadher and Schlenker,1999, Berrada et al., 1996, Meyer and Hofe, 2000, Nonobe and Ibaraki, 1998). Column generation was employed in nurse scheduling (Bard and Purnomo, 2005) using set covering-type models and integer programming. Knowledge based techniques have also been explored for solving nurse rostering problems (Beddoe and Petrovic, 2005, Lukman et al., 1991).

For an in-depth review of the nurse rostering literature, see (Burke et al. 2004). A brief summary follows. Miller et al. (1976) were the first to formally address the preference scheduling problem. Starting with an initial solution, they developed a greedy neighborhood search procedure to find local optima (Randhawa and Sitompul, 1993). More recently, metaheuristics, such as tabu search, have been designed for various nurse rostering problems. The distinguishing feature of these methods is their ability to escape local optima.

Starting with several initial solutions, GAs use crossover and mutation operators to generate pairs of improved solutions. This representation allowed the original problem to be viewed as a permutation problem, which is more suitable for GAs due to the nature of the exchange procedures. The column generation approach, an example of decomposition, uses the pattern-view formulation as a master problem and either heuristics or the shift-view formulation as sub problems to generate nurse rosters. In the vast majority of cases, the pattern-view formulation only includes demand constraints, which gives it the advantage of simplicity, although the number of columns grows exponentially with the length of the planning horizon. Alternatively, goal programming is a common methodology for dealing with soft constraints. In this approach, rules are prioritized and treated as goals or objectives to be satisfied. The optimization is carried out sequentially so as to ensure the achievement of the goal.

Constraint programming (CP) is also an AI technique that, unlike integer programming, does not make use of an explicit mathematical representation of the hard and soft constraints. Instead, the constraints are used to formulate propagation rules that reduce the search space. When constraint satisfaction is difficult to achieve, each constraint is assigned a different priority that is used to drive the search process. Solution quality is judged on the basis of priority satisfaction (Hadi and Jonathan, 2007).

NURSE ROSTERING PROBLEM

The terms scheduling and rostering are defined (Anthony, 1995) as follows:

- Scheduling is the allocation, subject to constraints, of resources to objects placed in space-time, in such a way as to minimize the total cost of the resources used.
- **Rostering** is the placing, subject to constraints, of resources into slots in a pattern.

Nurse rostering problem involves allocating the required workload to nurses subject to a number of constraints. Constraints are categorized into two groups; Hard and Soft Constraints, which vary with legal regulations and individual preferences.

- **Hard Constraints** are those that must be satisfied to obtain feasible solutions.
- **Soft Constraints** are typically time related constraints. They are desirable but not compulsory, and thus can be violated.

Without the loss of generality we discuss our contribution in the context of a specific nurse rostering problem as encountered by ORTEC in intensive care units in Dutch hospitals. This nurse rostering problem has the following characteristics.

1. Work requirements adhere to Dutch national legislation, and the collective labor agreements in force in Dutch hospitals.

2. The requests of the personnel are considered to be very important, and should be met as much as possible; These are represented as soft constraints.

3. It is not necessary to consider qualifications, as all personnel are highly qualified. Nurses still in training are disregarded in the original planning (and are added to the schedule afterwards).

4. The size of the department is rather small, but convenient for testing purposes.

We focus on creating weekly schedules for a ward with 15 nurses. The problem is to assigning a certain number of different types of shifts to 15 nurses in a ward within a scheduling period of 5 weeks. The required number of nurses on individual shifts for different days of the week is summarised in Table 1. The study is focussed on nurses with full-time contracts of 36 hours per week.

Shifts and personnel cover demand

There are 4 shift types in the problem. Each shift types covers 9 hours including one hour of resting time, except the night shift, which does not have resting time. So there are 8 actual working hours for each of these shift types.

In designing the shift sequences, we first consider shifts which are the most important or most difficult to schedule. In this problem, night shifts are the most important ones. This will result in three basic shift patterns presented in Table 2. These valid patterns will repeat for week 1 until 5.

Table 1. Shift Types and Demand during a Week

Shift	Start	End	Demand						
Туре	Time	Time	Μ	Т	W	Т	F	S	S
Early	07.00	16.00	3	3	3	3	3	2	2
Day	08.00	17.00	3	3	3	3	3	2	2
Late	14.00	23.00	3	3	3	3	3	2	2
Nigh	23.00	07.00	1	1	1	1	1	1	1
t									

Night = N Early = E Day = D Late = L

Table 2: Basic Night Shift Patterns

	М	Т	W	Т	F	S	S
Pattern A	Ν	Ν	-	-	-	-	-
Pattern B	-	-	N	Ν	-	-	-
Pattern C	-	-	-	-	Ν	N	Ν

The hard and soft constraints that need to be satisfied are described below respectively. Currently, hard constraint 11 and soft constraint such as 3b, 5b and 6b are not included in these studies.

Hard Constraints

The hard constraints listed below must be met in any circumstances otherwise the schedule is considered to be infeasible and unacceptable.

- 1) Demands need to be fulfilled
- 2) For each day, 1 nurse may start only one shift.
- 3) Within a scheduling period, a nurse is allowed to exceed the number of hours for which he/she is available for his/her department by at most 4 hours.
- 4) The maximum number of night shifts is 3 per period
- of 5 consecutive weeks.
- 5) A nurse must receive at least 2 weekends off duty

per 5 week period. A weekend off duty lasts 60 hours including Saturday 00:00 to Monday 04:00.

6) Following a series of at least 2 consecutive night shifts, a 42 hours rest is required.

7) During any period of 24 consecutive hours, at least 11 hours of rest is required. A night shift has to be followed by at least 14 hours rest. An exception is that once in a period of 21 days for 24 consecutive hours, the resting time may be reduced to 8 hours.

The number of consecutive night shifts is at most 3.

9) The number of consecutive shifts (workdays) is at most 6.

10) One of the full-time nurses requires not receiving any late shifts.

11) The maximum labour time per week is on average 36 hours over a period of 13 consecutive weeks if this period does not include work during night shifts.

Soft Constraints

Soft constraints, in the problem we are dealing with are listed below. Ideally these constraints should be satisfied as much as possible. However, in real world circumstances, it is usually necessary to violate some of these soft constraints. Depending on how strongly these soft constraints are desired (especially in comparison to other soft constraints).

1) For the period of Friday 23:00 to Monday 0:00, a nurse should have either no shifts or at least 2 shifts (Complete Weekend).

2) Avoid sequence of shifts with length of 1 for all nurses.

3a) For nurses with availability of 30-36 hours per week, the length of a series of *night* shifts should be within the range [2, 3]. It could be part of, but not before, another sequence of shifts.

3b) For nurses with availability of 0-30 hours per week, the length of a series of *night* shifts should be within the range [2, 3]. It could be part of, but not before, another sequence of shifts.

4) The rest after a series of *day*, *early* or *late* shifts is at least 2 days.

5a) For nurses with availability of 30-36 hours per week, the number of shifts is within the range [4, 5] per week.

5b) For nurses with availability of 0-30 hours per week, the number of shifts is within the range [2, 3] per week. 6a) For nurses with availability of 30-36 hours per week, the length of a series of shifts should be within the range of [4, 6].

6b) For nurses with availability of 0-30 hours per week, the length of a series of shifts should be within the range [2, 3].

7) For all nurse, the length of a series of *early* shifts should be within the range [2, 3]. It could be within another series of shifts.

8) For all nurse the length of a series of *late* shifts should be within the range of [2, 3]. It could be within another series of shifts.

9a) An early shift after a day shift should be avoided.

- 9b) An early shift after a late shift should be avoided.
- 9c) A *day* shift after a *late* shift should be avoided.
- 10) A night shift after an early shift should be avoided.

PROPOSED SOLUTION

Constraints listed in the previous section are defined at a very detailed time-resolution. In this form they can be quite overwhelming given the number of shifts in the planning horizon and the number of personnel to be scheduled. Following from the observation that there are only three feasible night-shift patterns that satisfy the hard constraints, as listed in Table 2, we proposed to identify feasible day-shifts in a similar way. This in effect represents abstraction from the detailed specification of hard constraints and the development of new semantical entities of feasible day- and nightpatterns to express the nurse-scheduling problem. In the context of Granular Computing we interpret this as granulation of constraints.

From the description of the shifts it is clear that the E, D and L type shifts are similar in terms of working hours and also in terms of work regulations that are applicable to them. By contrast, the night shifts represent a very different entity. We propose therefore that the nurse-scheduling problem may be expressed at a more abstract level using just two types of shifts daytime and night-time. Clearly this granulation of shift types implies introduction of hierarchical processing of schedules, since the final solution needs to be defined in terms of E, D, L and N shifts. Nevertheless, such a partitioning of the problem is advantageous because the large solution space of feasible schedules becomes significantly smaller for just two shift types and the post-processing task from day-time shifts into detailed E, D, L shifts is relatively easy.

Having defined the granular entities of shifts and patterns we proceed to formulate the nurse-scheduling problem as a recursive process with a time frame of one week. We postulate that a granulation of the scheduling horizon from individual days into weeks correlates closely with the granulation of constraints into patterns and consequently provides a natural simplification of the scheduling problem from the full-schedulinghorizon to a recursive-weekly-scheduling. Clearly, the search space that is pertinent to finding a weekly schedule is significantly smaller than the corresponding search space for the full-scheduling-horizon task.

The feasible schedules for week 1 for the granular nurse-scheduling problem can be enumerated relatively easily and can be seen as a new granular search space for the solutions for subsequent weeks. Since these schedules capture the essence of hard constraints and the requirements for personnel cover (which are predefined for the scheduling horizon) this set is exhaustive and can only be reduced by the introduction of additional constraints. As a result of the above granulations, the scheduling task becomes spanned by the relatively small vector of feasible patterns and schedules for week 1. The overall idea outlined above is to reduce the problem complexity by granulating the search space. The algorithm implementing this idea is outlined in the following:

1. Convert the problem space from {N,E,L,D,R} to a smaller space of {N,d,R}.

[The result of the granulation of the shift types is the reduction of the number of feasible shift patterns by several orders of magnitude. This point is illustrated in Figure 3. A large number of patterns of the type NNRRDDD, NNRRDLL, NNRRLLL, etc. are all represented by a single pattern NNRRddd. The saving implied by this granulation of shift types is pronounced even more strongly if one considers several weeks. If the number of detailed patterns represented by a single general pattern is K, then in a 5-week schedule one will have K^5 detailed patterns represented by a single general pattern. Notice that Pattern A in Table 2 reflects the same insight in the context of night shifts.]

2. Identify all the shift patterns with "0" cost for week 1 in the {N d R} space.

[This is carried out as offline processing of all hard and soft constraints. Although some of the hard constraints such as constraint 4 and 5 are specified in the context of 5 weeks scheduling horizon, they can be easily interpreted in the context of a oneweek scheduling with an appropriate additional constraint imposed onto subsequent weeks. The resulting set of 26 shift patterns is listed in Table 4.]

3. Within the space of feasible shift patterns for week 1 we identify sets of patterns that satisfy the personnel cover requirements, as specified in Table 3, which have cardinality equal to the number of nurses on the ward.

[In the case of our specific ward we have identified some 380 sets with cardinality 15 satisfying the personnel cover requirement of "9 9 9 9 9 6 6" for day-shifts and "1 1 1 1 1 1 1" for night-shifts. These 380 sets represent feasible schedules for week 1. It should be noted that by specifying different cardinality of the sets we can generate feasible schedules for different number of staff. Also we can easily take into account different requirements for personnel cover].

4. Extending the scheduling horizon from week "w" to "w+1" we identify which of the feasible 26 shift patterns need to be excluded for each specific pattern deployed in week "w".

[This step ensures that the hard constraints on the number of consecutive shifts on the interface of two weeks and the number of night shifts for a single nurse are satisfied. Note that this step reduces the search space of feasible schedules for week "w+1"]

5. Given the set of feasible schedules identified in point 3 above and the set of feasible patterns for the week "w+1" identified in point 4, we perform a search in this schedule space to find feasible schedules for week "w+1".

[The elimination of some of the patterns as a possible continuation after a specific pattern in week "w" (as highlighted in point 4) reduces the number of possible schedules that can be generated from this smaller set of patterns in week "w+1". Consequently some of the 380 schedules that were feasible in week "w" will not be feasible in week "w+1". However, an important conclusion is that a set of feasible schedules for week "w+1" is contained in the set of feasible schedules for week "w". This provides an upper limit on the extent of search that is needed to identify all feasible schedules in week "w+1". An example of a single feasible schedule for week "w+1" is given in Table 5]

6. The process of scheduling personnel for subsequent weeks is implemented by repeating steps 4 and 5 above until the set of feasible patterns is empty of the planning horizon has been reached..

Computational results

Figure 3 illustrates the granulation of the problem space and the consequent reduction of the set of feasible patterns.

Week 1	W	/eek 2	Wee	ek 3		
N N R R	ddd dd	R d d R R	d d d d	RR		
•••••						
	Week 1	Week 2		Week 3		.
N N N N	R R E E E R R E E E	E E R E D E E R E D	R R R R	E E E D E E D D	R R R R R R	
 N N 	RREED	D D R E E	RR	EEEC	O R R R	
 N N	R R D D D	D D R E E	R R	EEED	RRR	
	R R D L L	LLREE	RR	EEEC	O R R R	
NN	RRLLL	LLREE	R R	EEED	RRR	
				/		
f	Zero-Cost Sec or Specific d and night	quences ay shift shift)(Zero Sequer the gen and nig	-Cost nces for eric day ght shift	

Figure 3: Offline preparation Process

The constraints on the required personnel cover in the granulated problem space are represented in Table 3.

Τŧ	ab	le	3:	Demand	summar	ization
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Demand											
M T W T F S S											
d	9	9	9	9	9	6	6				
N											
	d = day N= Night										

Table 4 shows the 26 feasible shift patterns which were identified for the sample problem of a ward in a Duch hospital. Table 5 shows a representative 2-week schedule for 15 nurses that satisfies the problem constraints (i.e. it is a zero-cost schedule)..

Table 4: 26 common patterns

Pattern	Shift Sequence
P1	N N R R R d d
P2	N N R R d d d
P3	d d N N R R R
P4	R R R d N N N
P5	R R d d N N N
P6	d d R R N N N
P7	R d d R N N N
P8	d R R R N N N
P9	d R R d N N N
P10	R R d d R d d
P11	R d d R R d d
P12	R d d R d d d
P13	R d d d R d d
P14	R d d d d R R
P15	d R R R d d d
P16	d R d d R d d
P17	d R d d d R R
P18	d d R R R d d
P19	d d R d d R R
P20	d d d d R R R
P21	R R R d d d d
P22	R R d d d d d
P23	d R R d d d d
P24	d d R R d d d
P25	d d d d d R R
P26	d d d R R d d

As a rough guideline of the efficiency of the proposed algorithm we can report the following computational times on 1.64GHz PC with 448MB RAM:

a)generation of subsets, 0.156 sec

b) computation of 26 patterns, 0.242 sec

c) generation of week 1patterns : 3.954 secs

d) generation of the first 5 week schedule: 3600 sec

Table 5: A two-week schedule for 15 nurses

Nurse	Week1	Week2	Week1	Week2
No.	Pattern	Pattern	Sequences	Sequences
N1	P1	P12	NNRRRdd	RddRddd
N2	P3	P23	ddNNRRR	dddRRdd
N3	P4	P22	RRRdNNN	RRdddd
N4	P10	P1	RRddRdd	NNRRRdd
N5	P11	P15	RddRRdd	dRRRddd
N6	P11	P15	RddRRdd	dRRRddd
N7	P12	P17	RddRddd	dRdddRR
N8	P15	P5	dRRRddd	RRddNNN
N9	P17	P20	dRdddRR	ddddRRR
N10	P17	P3	dRdddRR	ddNNRRR
N11	P19	P14	ddRddRR	RddddRR
N12	P19	P14	ddRddRR	RdddRR
N13	P25	P19	ddddRR	ddddRRR
N14	P25	P19	ddddRR	ddRddRR
N15	P25	P20	ddddRR	ddRddRR
Total			9999966	9999966

CONCLUSION

Nurse rostering problem considered at the level of detailed time constraints and different types of dayshifts represents a very significant computational challenge. In this paper we propose an alternative granular formulation of the problem that reduces the size of the problem space and allows the replacement of the extended-time scheduling with the recursive application of a week-at-a-time scheduling process. The nested nature of sets of feasible schedules for consecutive weeks gives rise to a natural hierarchical algorithm for nurse rostering.

The study also shows the efficiency of identifying feasible patterns for subsequent weeks. Conceptually this approach can be generalized to non-zero cost pattern sets. Automating the nurse rostering problem can actually reduce the scheduling effort and time. It can also take care of all the constraints and give a quick evaluation of schedules. Information granulation was found to be very useful in providing a good quality of solutions by reducing the explorations of paths. This identification and extraction of good features used more explicitly to solve the problem and hence to reduce the search space.

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GRANULAR MODELLING OF EXAM TO SLOT ALLOCATION

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Information granulation, conflict chains, spread matrix, pre-processing, exam-to-slot allocation.

ABSTRACT

In this paper, we are introducing a new method of granular exam-to-slot allocation based on the preprocessing of the basic student-exam information into a more abstract (granulated) entity of conflict chains. Since the conflict chains are designed to capture the mutual dependencies between exams, they enable us to reason about the exam-to-slot allocation for all exams in a chain rather than just one exam at-a-time. The initial exam-to-slot allocation, generated through the processing of conflict chains, is then refined by considering the spread of the exams in the examination session so as to minimize the appropriately defined cost function. The granular pre-processing of problem data has been shown to enhance the efficiency of the exam scheduling task and has led to the identification of very competitive exam schedules.

INTRODUCTION

Exam timetabling represents a difficult computational problem due to the strong inter-dependencies between exams caused by the many-to-many relationship between students and exams. Timetabling researchers have investigated various methods of exploring the large combinatorial search space to generate timetables. These methods were typically formalized as heuristic assignment algorithms. However, it has been observed that no single heuristic that can be used to solve all timetabling problems because of the incorporation of problem-specific features in the heuristics (Burke et. al, 1994). In their survey (Qu et. al, 2006) point to the specialization of the timetabling research into sub-areas of educational timetabling, nurse scheduling, transport scheduling, sports timetabling, etc. However, according to the authors the most studied and researched timetabling problem is the educational timetabling and in particular, exam timetabling. The survey highlights families of related heuristics deployed in the solution of timetabling problems which include: graph heuristics, meta-heuristics, constraint based methods, multi-criteria techniques, hybridizations, and methods that focus on the investigation of neighbourhoods in the solution space.

In exam timetabling problems, the constraints are normally different from one institution to the other, which makes it difficult to define the "standard timetabling problem". However, at a general level the exam timetabling can be thought of as a process of ensuring that all students are able to take their exams and that the schedule of examinations for each student is designed so as to maximize the gap between consecutive examinations.

In a more formal way, the timetabling literature defines two types of constraints:

a) Hard Constraints

These are the constraints that must be satisfied at all times. The principal hard constraint is the requirement that not a single student is enrolled for two exams scheduled in the same timeslot. Another hard constraint that needs to be obeyed is the room capacity; i.e. there must be enough spaces in a room to accommodate all students taking a given exam. A timetable, which satisfies hard constraints, is called a feasible timetable.

b) Soft Constraints

Soft Constraints are not critical but their satisfaction is beneficial to students and/or the institution. An example of a soft constraint is the requirement to spread out exams taken by individual students so that they have sufficient revision time between the exams they are enrolled on. Typically one cannot satisfy all soft constraints thus there is a need for a performance function measuring the degree of satisfaction of these constraints.

Since the complexity of the timetabling methods reported in the literature seems to originate from the many-to-many relationship between the students and the exams we are proposing, in this paper, to cast the timetabling problem as a granular modeling problem in which the detailed student-exam data is pre-processed into some granular entities before these are used for expressing the timetabling problem itself. Apart from generating feasible timetable, our focus is to produce a good quality timetable, which satisfies the soft constraints to the greatest possible extent. To demonstrate the general applicability of the proposed granular modeling we produce solutions for both uncapacitated and capacitated versions of the timetabling problems, reported in the literature. In is worth noting here that the capacitated version of the exam timetabling problem means that the problem is subject to additional constraints on total room capacity in each timeslot. Consequently the expected quality of the timetables, as measured by the value of the cost function, is necessarily inferior compared to the uncapacitated version of the problem. For this paper, we have used the University of Nottingham Semester 1, 1994 dataset that can be downloaded from the URL: http://www.cs.nott.ac.uk/~rxq/files/Nott.zip.

The quality of the timetable is measured using the cost function originally proposed by Carter (Carter et al, 1996) and also used by other researchers (Burke et al, 2004). The function is:

$$\frac{1}{T} \sum_{i=1}^{N} \sum_{j=i+1}^{N} s_{ij} w_{|\rm pj - pi|}$$
(1)

where *N* is the number of exams, s_{ij} is the number of students enrolled in both exam *i* and *j*, *pj* is the time slot where exam *j* is scheduled, *pi* is the time slot where exam *i* is scheduled and T is the total number of students. Based on this cost function, a student taking 2 exams that are t slots apart, where t={1, 2, 3, 4, 5, 6}, will give rise to the costs of 16, 8, 4, 2, 1 and 0 respectively.

We also used another cost function that considered only the number of students having exams on the same day and students having exams separated by overnight break.

INFORMATION GRANULATION IN THE ALGORITHM

The proposed granular modeling of the timetabling problem starts with the abstraction of the detailed student-exam data into an aggregated (granular) entity describing mutual dependence of individual exams (arising from students taking both exams). We refer to this granular construct as a "conflict chain". The rationale for building conflict chains is that once an interrelated set of exams has been identified, allocating any of the exams in the conflict chain to a specific time slot implies a unique relative allocation of all other exams in the conflict chain to their respective time slots. In other words, we take advantage of the fact that the potential conflict between exams does not depend on the absolute allocation of exams to time slots. On the other hand the all-important relative allocation of exams to time slots is captured within one entity thus making any subsequent reassignment very straightforward. The generation of conflict chains is accomplished as a simple pre-processing of the original problem data. The resulting re-definition of the timetabling problem, away from the allocation of individual exams to time slots and towards the allocation of conflict chains to the corresponding sets of time slots is rooted in the Granular Computing research (Bargiela, et. al, 2002, 2008).

The first pre-processing step is to determine potential clashes between examinations and to count the number of students that cause these clashes. Since the potential clashes (unlike the actual ones) do not depend on the subsequent allocation of exams to time slots they represent useful information granules that can be utilized in the timetabling process. Based on these information granules we determine the minimum number of time slots that are necessary for timetabling the given set of examinations. We refer to this stage as the construction of conflict chains. The algorithm deployed at this stage can be summarized as follows:

- 1. Initiate the algorithm by allocating all exams to time slot one.
- 2. Select the first exam as "current" and initiate the counter for the current conflict chain.
- 3. Label the current exam as "allocated to the current chain" and note all the exams that are in potential conflict with the current exam.
- 4. If the list of potentially conflicting exams is nonempty, re-allocate those exams to the next available time slot. Otherwise label the current chain as complete and proceed to Step 6.
- 5. If the list of potentially conflicting exams is nonempty, select the first exam from the list and repeat from Step 3 with the currently selected exam.
- 6. Check if all exams allocated at Step 1 are belonging to one of the conflict chains; if YES than the algorithm terminates; if NO, then the conflict chain counter is incremented and the unallocated exam is taken as "current" for processing starting from Step 3.

The outcome of the above algorithm is a set of conflict chains that represent mutually dependent exams that need to be scheduled in different time slots so as to avoid violation of hard constraints. However, the algorithm implies that it is possible to have one exam belonging to more than one conflict chain (albeit the algorithm will ensure that the allocation of this exam to time slot is consistent in both chains). For this reason we perform additional step of merging these conflict chains, which happen to have common exams. The merged conflict chains represent independent subsets of the examination set that can be dealt with one-at-a-time.

It is worth noting that the length of the conflict chain, measured as the number of necessary time slots to schedule the exams in this chain, provides an immediate indication of the difficulty of the specific timetabling task. If the number of available time slots is equal or only slightly greater than the length of the longest conflict chain than the problem is heavily constrained and we might expect that the quality of the resulting timetable, measured by the cost function, will be low. On the other hand, if the number of the available time slots is significantly greater than the length of the longest conflict chain than we can expect high quality (low cost) solutions. Of course, if the number of available time slots is less than the length of the conflict chain then the timetabling problem is infeasible.

Consequently, the information granule of conflict chain provides a useful insight into the timetabling problem from a more general perspective compared to the one afforded by considering individual exams.

	1	2	3	4	5	6	7
309	11	0	11	0	0	0	0
310	2	0	0	0	0	0	0
311	7	0	0	0	7	0	0
312	6	0	0	0	0	0	0
313	1	0	0	0	0	0	0
314	1	0	1	0	0	0	0
315	3	0	0	0	0	0	0
316	19	0	19	0	0	0	0
317	0	0	0	0	0	0	1
318	6	0	0	0	0	0	0
319	11	0	0	0	0	0	0
320	10	0	10	0	0	0	0
321	0	0	0	0	0	0	2
322	11	0	0	0	0	0	0
323	0	0	0	0	0	8	0
324	10	0	10	0	0	0	0
325	11	0	11	0	0	0	0
326	2	0	0	0	0	0	0
327	9	0	0	0	0	0	0
	:	:	:	:	:	:	:
439	4	0	4	0	0	0	0
440	1	0	0	0	0	0	1
441	13	0	13	0	0	0	0

Figure 1: Conflict Chains Before Merging

Figure 1 illustrates a representative section of the output of the conflict chain generation algorithm. The chain label is given in the first row and the exam number is indicated in the first column. It can be seen that conflict chains 1, 3 and 7 share some of the exams between themselves. For example, exam 309 is shared between conflict chain 1 and 3, exam 311 is shared between conflict chain 1 and 5 and exam 440 is shared between conflict chains 1 and 7. This means that conflict chains 1, 3 and 7 can be justifiably merged into one conflict chain. It is worth noting that merging conflict chains 1 and 7 implies that the merged conflict chain will include also exams 317 and 321 even if they appeared only in conflict chain 7.

Figure 2, illustrates the resulting merged conflict chain under the chain label 1. Conflict chains 2, 4 and 6 are unaffected by this post processing as they happen not to have any common exams with those from chain 1. In particular, it is worth noting that the exam 323 is assigned to time slot 8 in conflict chain 6 but, since it is not in conflict with any of the exams in chain 1, it has label 0 in the merged conflict chain 1.

	1	2	3	4	5	6	7
309	11	0	0	0	0	0	0
310	2	0	0	0	0	0	0
311	7	0	0	0	0	0	0
212	1	0	0	0	0	0	0
312	6	0	0	0	0	0	0
313	1	0	0	0	0	0	0
314	1	0	0	0	0	0	0
315	3	0	0	0	0	0	0
316	19	0	0	0	0	0	0
317	1	0	0	0	0	0	0
318	6	0	0	0	0	0	0
319	11	0	0	0	0	0	0
320	10	0	0	0	0	0	0
321	2	0	0	0	0	0	0
322	11	0	0	0	0	0	0
323	0	0	0	0	0	8	0
324	10	0	0	0	0	0	0
325	11	0	0	0	0	0	0
326	2	0	0	0	0	0	0
327	9	0	0	0	0	0	0
:	:	:	:	:	:	:	:
439	4	0	0	0	0	0	0
440	1	0	0	0	0	0	0
441	13	0	0	0	0	0	0

Figure 2: Conflict Chains After Merging

Besides generating the independent conflict chains, as outlined above, we evaluate the number of students who take exams allocated to time slots that are 1, 2, ..., 5 time slots apart. Since we are dealing with information granules that represent a potential conflict between all exams in one time slot and all exams in another time slot, regardless of what are the actual time slot numbers, we create a framework for efficient optimization of the cost function (quality of the timetable). In what follows we will describe the proposed scheme for re-numbering of the time slots using the background knowledge about the structure of the cost function. We refer to this optimization stage as maximizing the spread of examinations.

The spread information is represented as an [sxs] matrix, where s is a number of time slots in the given timetabling problem. Figure 3 illustrates a section, representing the first six time slots, of the spread matrix evaluated for the Nottingham Dataset. We can observe that there are 1454 students who take an exam in time slot 1 and 2, 1360 students taking exams in time slot 1 and 3, etc. Clearly, the spread matrix is symmetrical

with diagonal elements being omitted from the calculation.

Taking into account the format of the cost function that assigns the weight "16" to the exam spread of 1 (i.e. entries in the spread matrix (1,2), (2,3), (3,4) etc.) and assigns weight "8" to the exam spread of 2 (i.e. entries in the spread matrix (1,3), (2,4), (3,5), etc.), and so on, we can reformulate the task of optimization of the exam spread as a task of re-arranging the time slots so as to achieve the smallest sum of elements on the first minor diagonal in the re-arranged spread matrix. Taking this method to a logical conclusion we aim at making sure that some particularly large numbers in the spread matrix are shifted to minor diagonals that are of order 6 or above (thus not imposing penalties in the cost function). Of course, re-numbering of time slots is subject to strong mutual dependencies so one needs to define some compromise strategies.

	1	2	3	4	5	6
1	0	1454	1360	1717	1276	1006
2	1454	0	1355	1634	1085	997
3	1360	1355	0	1392	1158	947
4	1717	1634	1392	0	1529	1446
5	1276	1085	1158	1529	0	1120
6	1006	997	947	1446	1120	0

Figure 3: Initial Ordering of the Spread Matrix for the First 6 Slots from the Nottingham Dataset Based on the Largest Degree (LD) Decreasing Ordering

We propose here two strategies for optimization of the exam spread named as Method 1 and Method 2. A brief explanation of each method is given below:

Method 1

The first method is focused on extracting the smallest element in each row of the original spread matrix and re-numbering the relevant time slots so as to place the smallest element on the first minor diagonal. While implementing such re-numbering it is possible that higher order minor diagonals will have some greater elements associated with them. However, if the primary concern is to minimize the number of adjacent exams the method provides the optimum solution.

Method 2

The second method takes another approach of identifying the smallest elements in both rows and columns and shifting them towards the first minor diagonal. This corresponds to arranging simultaneously from the first slot and from the last slot towards the middle one. It turns out that by taking this approach a more balanced re-numbering is achieved that attempts to minimize the sum of higher minor diagonals.

The first six rows-columns of the re-numbered spread matrix using Method 1 and 2 are shown in Figure 4 and Figure 5 respectively. However, one needs to remember that some of the rows-columns represented in Figures 4 and 5 do not appear in Figure 6 because they had their corresponding time slot number greater than 6. Nevertheless the sample spread matrices serve to illustrate the main characteristics of the two methods.

	1	2	3	4	5	6
1	0	1006	1360	1276	1454	1717
2	1006	0	947	1120	997	1446
3	1360	947	0	1158	1355	1392
4	1276	1120	1158	0	1085	1529
5	1454	997	1355	1085	0	1634
6	1717	1446	1392	1529	1634	0

Figure 4: The New Arrangements of the Initial Ordering of the Spread Matrix after Applying Method 1

	1	2	3	4	5	6
1	0	1006	1717	1360	1454	1276
2	1006	0	1446	947	997	1120
3	1717	1446	0	1392	1634	1529
4	1360	947	1392	0	1355	1158
5	1454	997	1634	1355	0	1085
6	1276	1120	1529	1158	1085	0

Figure 5: The New Arrangements of the Initial Ordering of the Spread Matrix after Applying Method 2

It is worth highlighting here that our proposed solution to the timetabling problem is fundamentally different from the previous solutions based on consideration of one-exam-at-a-time (Lewis, 2008). By pre-processing the original data into suitable information granules we were able to re-formulate the problem as an optimization of minor traces of the spread matrix.

COMPUTATIONAL RESULTS

The proposed method has been evaluated on a real-life dataset representing examinations at the University of Nottingham scheduled during the 1994-5 autumn semester (Table 1).

Table 1: University of Nottingham Dataset (Nott), Semester 1, 1994-1995 Used in Our Experiment

Dataset	Number of	Number of	Number of	Conflict density
	students	exams	enrollments	
Nott	7896	800	33997	0.03

In order to ensure that the conflict chains are produced as efficiently as possible, we have pre-ordered the exams using the Largest Degree (LD) method (i.e. gave priority to the exams that have the largest number of conflicting exams). The granulation of this data set into conflict chains resulted in the identification of 18 time slots as the minimum number required for the satisfaction of hard constraints. The cost function (1) evaluated on the merged conflict chains without- and with the optimization of the exam spread using Method 1 and Method 2 are presented in Table 2:

Table 2: Cost Functions Before and After Considering the Spread Information for the Uncapacitated Nott Dataset.

No of slots	18
Cost Function with original ordering of time	43.91
slots	
Cost Function After Rearrangement of slots	
using Method 1	29.03
Improvement Percentage (%)	33.89
Cost Function After Rearrangement of slots	
using Method 2	24.18
Improvement Percentage (%)	44.93

It is clear that the optimization of the spread matrix by re-numbering of the exam slots leads to a significant improvement of the cost function. It is worth noting here that we are considering the smallest number of time slots that allows generation of the feasible schedule. As such, the cost function is necessarily large because there is little room for maneuver with moving time slots around.

An alternative version of the Nottingham examscheduling problem involves on one hand a relaxation of the constraint on the number of time slots from 18 to 23 and the introduction of an additional constraint on the number of students taking exams in any of the time slots (maximum number 1550). Using the same cost function (1) and evaluating the results for the original ordering of time slots and the optimized ordering using Method 1 and 2 we obtain results reported in Table 3.

Table 3: Cost Functions Before and After Considering the Spread Information for the Capacitated Nott Dataset.

No of slots	23
Cost Function with original ordering of time	22.51
slots	
Cost Function After Rearrangement of slots	
using Method 1	21.29
Improvement Percentage (%)	5.42
Cost Function After Rearrangement of slots	
using Method 2	19.61
Improvement Percentage (%)	12.88

The inspection of the spread matrix generated by both methods reveals that the first method tends to overemphasise the selection of small spread values on the first minor diagonal and by the time the optimisation gets to dealing with few remaining time slots the capacity constraints forces it to leave the high spread values on the bottom-right section of the first minor diagonal. By contrast the Method 2 takes a more balanced approach to optimizing the spread values and, in doing so, is less affected by the capacity constraint, thus producing lower overall cost.

The capacitated Nottingham exam-scheduling problem has been also evaluated using an alternative cost function as proposed in (Qu et al, 2006). In this version of the problem the objective is to minimize adjacent exams on the same day and overnight. By extracting information from the spread matrix, the values obtained are 3565 for adjacent periods and 1536 for overnights, in the original ordering of time slots. If we quantify this result using a function similar to (1) but defined only on the adjacent time slots we have: (3565 + 1536) * 16 /7896, which equals to 10.34. Performing similar evaluation for the re-numbered time slots generated using Method 1 and 2 we obtain 6.13 and 11.60 respectively, as reported in Table 4:

Table 4: Cost Functions For Nott Dataset Based onNott94b Evaluation.

Method	Adjacent Periods	Overnights	Penalty (Violations of the first constraint Using Carter et al, 1996)
Initial Ordering	3565	1536	10.34
Method 1	1729	1298	6.13
Method 2	3260	2465	11.60

The results reported in Table 4 are consistent with the nature of the Method 1 and 2. Since the cost function penalizes only the adjacent examinations the optimization implemented by Method 1 provides an optimal choice (resulting in the overall cost of 6.13). The more balanced approach to the optimization of the spread afforded by Method 2 does not produce any advantage here since it does not reflect the narrow focus of the cost function. Consequently the cost associated with Method 2 is not only worse than the one obtained with Method 1 but also is worse than the one for the original ordering.

In order to enable a cross-comparison of the results generated by granular modeling with those produced using alternative approaches, we have archived complete solutions reported here at URL http://www.intelligentmodelling.org.uk/UNMC/timetabl ing.html.

CONCLUSION

Information granulation is a powerful methodological approach to emphasizing the relevant information embedded implicitly in the raw data. Granular models of the problem that are built on such aggregated (granular) data can be much simpler in terms of computational complexity and indeed can lead to simple analytical or combinatorial optimization.

We have shown that by capturing the persistent feature of potential conflicts (as opposed to actual) in the conflict chain information granule one can construct a much simpler model of the exam-scheduling task. Such a granular model is then amenable to optimization by minimization of the trace of minor diagonals of the exam spread matrix.

Numerical experiments conducted on the Nottingham Dataset confirmed the insights about the potential of granular modeling of the exam scheduling problem and have delivered very competitive exam schedules.

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