MODEL-BASED APPROACH TO STUDY HOT ROLLING MILLS WITH DATA FARMING

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KEYWORDS

Model-based simulations, parameter studies, high-performance computing, rolling technology design.

ABSTRACT

The paper describes a computer system for simulating metallurgical rolling processes that consist of multiple steps, each of which is performed by a different type of devices. Both devices and processed materials are described with models, which can be dynamically reconfigured between simulation runs to study different device and environment configurations. Such an approach is especially crucial in technology design based on multi-iterative optimization procedures, for which an objective function uses computationally intensive algorithms. Due to the approach proposed in this paper, in the first stage of optimization more general and coarse models can be applied characterized by lower predictive capabilities and higher computational efficiency. Afterwards, when the optimization procedure finds a solution close to the optimal one, very detailed models can be used to obtain high quality solutions in the last few steps of calculations. To achieve such an objective a hybrid computer system able to use High Performance Computing (HPC) infrastructures was designed and implemented. The details of proposed approach are described, which is followed by presentation of a data farming platform responsible for distribution of complex numerical simulations onto various computer clusters. Finally, a concrete use case of a hot rolling mill is presented and analyzed.

INTRODUCTION

Computer simulation is an essential tool used to verify a stated hypothesis faster and in a more cost-effective way compared with physical experiments in various computational-oriented science fields and in the industry. Metallurgy and metal forming processes, e.g. rolling and cooling, are representative examples of successful simulation applications. Attaining desired mechanical properties of hot rolled Advanced High Strength Steels (AHSS) and Ultra High Strength Steels (UHSS) strips (which are utilized in many branches of industry, e.g. the automobile one) requires implementation of thermo-mechanical schemes, in terms of time/temperature/deformation along the hot rolling process. Such a complex metallurgical process can be realized in a cost-effective way by simulating hot rolling strip mills consisting of multiple devices with distinct configurations.

Data farming (Horne and Seichter 2014) is an example of a methodology, which combines data exploration and analysis methods with efficient exploitation of modern computational infrastructures such as HPC computer clusters. Its main goal is to increase data volume in a systematic manner in virtual experiments by executing the same simulation many times with different input parameter values. The collected results are then used to gain knowledge about the studied processes.

Advancements in computer hardware in recent years have significantly decreased the time required to run simulations and enabled refinement of simulation models with regard to their complexity (Rauch 2012). Besides accelerating simulations, the modern high-performance computer clusters are capable of processing much more data in a given time interval than ever before. As a result, data farming experiments containing dozens of simulation cases can be finally conducted during the time, which is satisfactory for the industry.

However, harnessing computer clusters to execute complex numerical simulations is a challenging task when dealing with large-scale simulation-based experiments. Neither remote access nor unified interface nor provision of abstraction layers are typically offered by current queuing systems to defining computer experiments as a collection of simulation runs with different input parameter values, like different material models or device configurations. Thus, in the presented work, a higher-level platform, called Scalarm, for data farming computing (Król and Kitowski 2016) has been used.

The above mentioned challenges justified the development of a model-based computer system (VirtRoll) in the framework of the Research Fund for Coal and Steel (RFCS) VirtROLL project, which combines numerical simulations, multiscale modeling, meta-modelling, inverse analysis and optimization techniques to minimize costs of design of production technologies and to optimize semi- and final product properties. In a nutshell, the main objective of the project is to combine a model database and inverse solution coupled with optimization techniques in one comprehensive computer system oriented on enabling domain experts to create and simulate a virtual hot rolling mill (Rauch et al. 2012) equipped with selected

Proceedings 30th European Conference on Modelling and
Simulation ©ECMS Thorsten Claus, Frank Herrmann,
Michael Manitz, Oliver Rose (Editors)
ISBN: 978-0-9932440-2-5 / ISBN: 978-0-9932440-3-2 (CD)

devices.

The rest of the paper is organized as follows: Section 2 specifies the problem, which is solved by the proposed system, Section 3 contains an overview of the proposed system, its architecture and differentiating features, Section 4 describes the system's evaluation in the context of hot rolling mills simulations and Section 5 concludes the paper.

PROBLEM STATEMENT

Let us assume we have a multi-phase metallurgical process to simulate, in which each phase is conducted by a different device. Each device is modelled by a different numerical procedure with multiple configuration options, which influence the results. The processed material is described by constant properties and models, including description of rheology and microstructure evolution. The main problem is to determine the optimal parameters of production devices, which lead to the desired output, i.e. to semi- and final products with specified thermo-mechanical properties. Moreover, the goal is to achieve the answer in reasonable time, which could be accepted also by the industrial practice. Therefore the main objective of the work is to design and implement such mechanisms, which allow for:

- replacing numerical models dynamically between subsequent iterations of an optimization procedure,
- facilitating usage of modern HPC infrastructures in a seamless manner.

PROPOSED SOLUTION

Studying rolling-related processes, by building a virtual hot rolling mill can be described as a multi-step workflow involving: 1) design of a virtual hot rolling mill, 2) design of the computational experiment, 3) simulation of the rolling process with the parameter study approach, and 4) output data exploration with optimization and sensitivity analysis methods to discover relationships between the hot rolling mill parameters and the obtained thermo-mechanical properties in the final product. An overview of the proposed system is depicted in Figure 1. There are three main elements of this solution: a virtual workbench where a hot rolling mill is designed and configured; middleware which is responsible for simulation scheduling onto remote HPC computer clusters; and numerical simulations actually executed on the clusters.

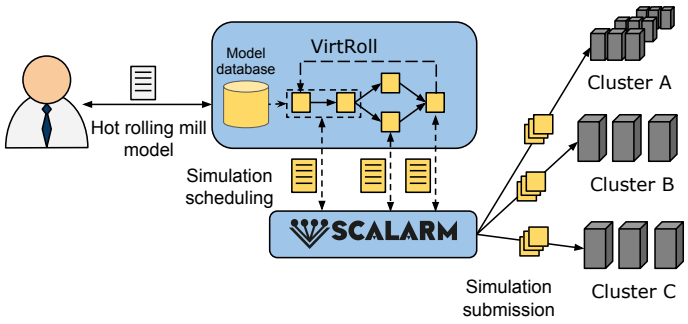

Figure 1: Overview of VirtRoll Integration with the Scalarm Platform.

Design of Hot Rolling Mill – Web-Based VirtRoll Module

The functionality leading to design a new rolling mill is covered by a web-based module, which, in connection with a database, allows for efficient management of production devices, materials and models. Due to the flexibility-oriented design of the database a schema-less document-oriented MongoDB engine was used. This choice was dictated by the necessity to keep the flexible data model of the process supporting addition of new materials and devices characterized by different parameters.

The hot rolling mill design is prepared with a virtual workplace, which enables the users to either prepare a hot rolling mill design from the scratch or select and fine-tune an existing project of a rolling mill common scheme. Moreover, the user can upload new material or devices models and use them in the simulation process. At first, the user selects devices, their placement on the rolling line and configuration parameters. Afterwards, the material to be processed and its models are selected.

The database includes descriptions of different kinds of steels, characterized by grade, name and chemical composition, which can be used further by numerical models.

Flexibility of the VirtRoll system enables the users to add new material models through the graphical user interface (GUI). Therefore, a generic library with abstract classes organized in a multi-level hierarchy for direct inheritance was created. The classes already implemented are as follows:

- `Model` – a root class of the whole hierarchy, containing abstract method for the main algorithmic part of the model. The method is implemented by each model separately. The main attributes of this class are collection of parameters and map of the parameters, which allow to manage model parameters dynamically.
- `RheologicalModel` – the main class for rheological models containing definition of fundamental models for plastic metal forming. Specific models like `HenselSpittel`, `CEMEF` or `Sellars` inherit from this class and define their own parameters as well as a method for numerical calculations,
- `MicrostructureEvolution` – the abstract class allowing definition of derived classes responsible for calculation of grain growth, static `StaticRecrystallizationModel`, dynamic `DynamicRecrystallizationModel` and metadynamic `MetadynamicRecrystallizationModel` recrystallization. The simulations of microstructure evolution are managed by `MicrostructureEvolutionLogic`, which aggregates all other models. The logic class can be also inherited and implemented specifically for new material grades.
- `PhaseTransformation` – defines basic functionality for classes responsible for simulation of four main phase transformations i.e. `FerriteTransformationModel`, `PearliteTransformationModel`, `BainiteTransformationModel` and

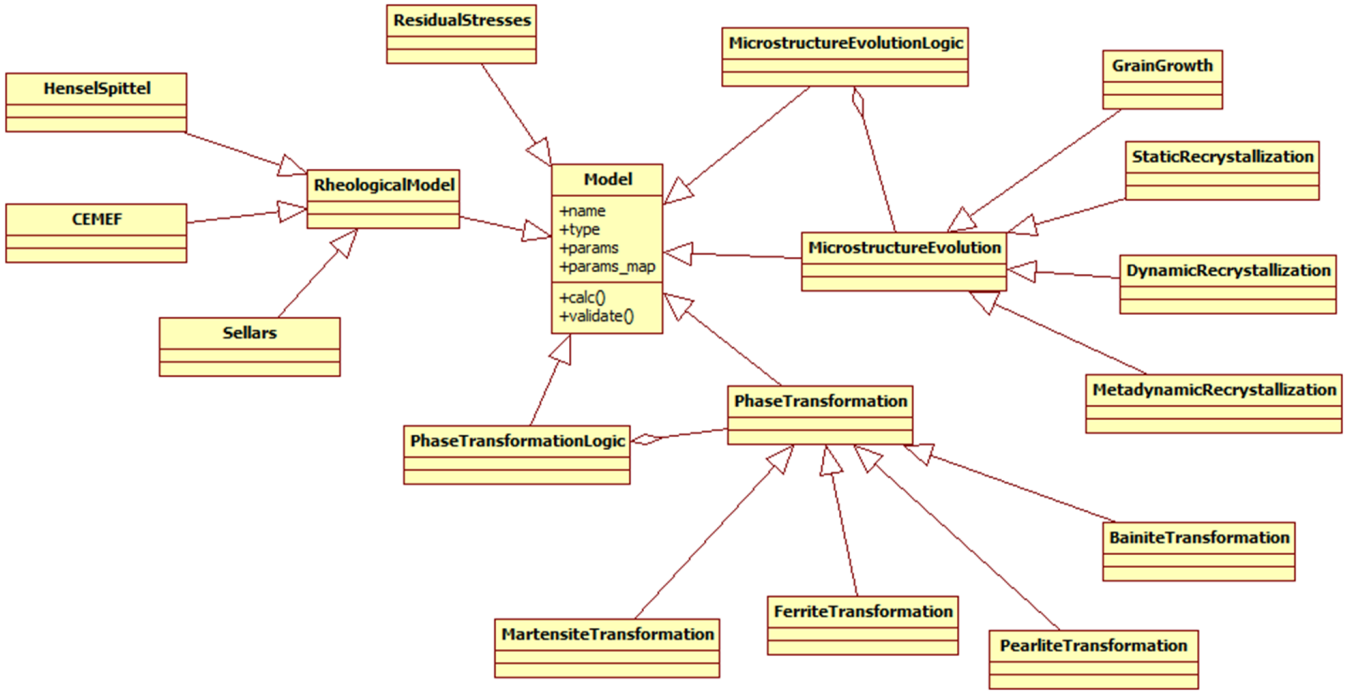

Figure 2: Module Containing Classes Used in Modeling of Hot Rolling.

`MartensiteTransformationModel`. Similarly to microstructure evolution in the case of phase transformation the separated class, dedicated to management of phase transformation logic, was implemented (`PhaseTransformationLogicModel`).

The implemented models in the form of different classes of the presented hierarchy were described in (Pietrzyk et al. 2015) in more details.

Design of Computational Experiment with Scalarm Platform

In the presented work, verification and validation of semi- and final products properties obtained with the designed virtual hot rolling mill is conducted by applying the data farming methodology. The user prepares a parameter space involving formed material parameters, devices configuration in the rolling mill and environmental conditions. Each data point in the parameter space describes a distinct simulation case of a virtual hot rolling mill. Therefore each data point can be executed in parallel using distributed HPC computer clusters. Simulation results are available online to visualize progress of any given simulation. This functionality is attained by integrating the VirtRoll system with the Scalarm platform. Scalarm is a tool designed to support the management of data farming experiments, including input parameter space specification, execution, and results collection. Scalarm provides two user interfaces: graphical user interface in form of a web-based application and HTTP-based API. The graphical user interface is oriented towards the users who currently run their simulation codes manually on various infrastructures and would like to facilitate this process. The HTTP-based API is exposed to support integration of third-party tools with Scalarm using the common JSON data representation format. Hence, the integration of the VirtRoll system with Scalarm is based on this approach as depicted in Figure 1. The following list describes the most important methods of the API for computation delegation from the VirtRoll system to actual computational infrastructure:

(1) registering a simulation scenario – it is a prerequisite of conducting a parameter study experiment with Scalarm; in the presented case the VirtRoll system registers simulation binaries/codes and description of simulation input parameters for each hot rolling process phase,
(2) starting a new simulation experiment – arguments of this method include identification of a previously registered simulation scenario and input space specification, i.e. parametrization types and specific attributes for each selected parametrization type, e.g. a model describing material to be processed or configuration options for a simulated device,
(3) scheduling computations – the user can specify how much computing power and from which cluster should be used to execute simulations,
(4) getting information about experiments progress – at any given time the user can check how many simulation runs are running and how many of them were completed,
(5) download experiment results – an integrated third-party tool can download results of the already completed simulation runs, e.g. in form of a CSV file, to enable further analysis in the VirtRoll system,
(6) extending an experiment – based on the conducted results exploration, it may be necessary to explore some additional parameter space to study some interesting cases, not included previously,
(7) stopping an experiment – when all simulation runs were

completed, the experiment can be stopped and marked as historical; in such a case the experiment results are stored in the platform and can be explored.

The open-source Scalarm platform supports simulation execution on different types of computing infrastructures including: computer clusters, grids and clouds, by using abstraction of computing tasks, infrastructure facades and infrastructure credentials (Król et al. 2014b). It is available online (http://www.scalarm.com), hence the third party tools can be integrated and used in any research. Scalarm was started as a module for data farming within the EDA EUSAS project (Kvassay et al. 2012), where it was was used to enhance the training process of security forces through evaluating strategies used during missions. Since then, Scalarm has been used in other scientific disciplines including: computational chemistry (Król et al. 2014a), metallurgy (Rauch et al. 2015), and computer science (Funika et al. 2015).

Numerical Simulations on HPC Computer Clusters

The main part of the system is encapsulated in separated computational module responsible for numerical modelling of macro and micro properties of material. The macro scale simulations of temperatures are realized by using FE method coupled with mechanical and microstructural models.

Mechanical Model.
Originally developed finite element (FE) simulation model (Pietrzyk 2000) was used to calculate strains, stresses, forces, torques and temperatures. Even if a simple stationary FE model with a coarse mesh is used in simulations of metal flow in rolling, the computing time for one pass is about 2-3 minutes. Since a lot of passes have to be simulated to determine one value of the objective function, it is useful to search for alternative models, which can accelerate optimization. Application of the metamodel approach is such an alternative. A metamodel of the process or phenomenon is a certain abstraction created on the basis of the lower level model developed using mathematical techniques. Thus, any approximation of the basic model, which gives reasonably realistic description of the process, can be considered as a metamodel, which allows for significant decrease of the computing time.

Various techniques can be used to build metamodels. Artificial Intelligence (AI) methods, in particular Artificial Neural Networks (ANN), are the most common. When the cost of computations for training data is not so high and large training data sets can be created, application of the ANN is efficient and even very complex relationships can be accurately described by the metamodel. Contrary, when the FE method is used to generate training data, the costs of computations of one set of data are high and other metamodelling techniques should be searched. The surface response method was used in the present work to calculate mechanical parameters including strains, stresses, forces and torques. An additional advantage was made of the fact that the material flow stress is the main factor, which decides about the accuracy of calculation of force parameters and influence of the geometrical parameters is of lesser importance. Therefore, the emphasis was put on accurate identification of the flow stress model. Plastometric tests were performed for each material from the database and the flow stress models were identified using the inverse analysis (Szeliga et al. 2006). The relation between the flow stress (σ_p) and the average pressure (p_{av}) in rolling has to account for so called friction hill and this relation was described by the surface response method. The metamodel follows the idea of Sims (Sims 1954), who introduced a coefficient Q representing the average pressure-to-flow stress ratio ($Q = p_{av}/(a\sigma_p)$, where $a = 2/\sqrt{3}$). Large number of calculations was performed using FE program (Pietrzyk 2000) for different reductions (ε), roll radius (R) and friction coefficients (μ). This data were used to find polynomial relation describing the function $Q = f(\varepsilon, R, \mu)$. However, the sensitivity analysis has shown that the effect of the design variables can be combined together by introduction of one variable $\xi = \mu/\Delta$, where Δ is the shape factor defined as h_{av}/l_d, $h_{av} = (h_1 + h_2)/2$ is an average thickness, $l_d = \sqrt{Rh_1\varepsilon}$ is the length of the arc of contact. Several FE simulations were performed for various process parameters and it was found in (Szeliga et al. 2011) that for a wide range of strip thicknesses and reductions the relationship between Q and ξ is linear. In consequence, the following equation was obtained by approximation of results of the FE simulations:

$$F = \sigma_p l_d w \left(1 + 0.572\frac{\mu}{\Delta}\right) \tag{1}$$

where: w - width of the strip, F - rolling force.

Several flow stress models are implemented in the system, described in (Pietrzyk et al. 2015) and not reported here. The Hensel-Spittel model (Hensel and Spittel 1979) was used in the case study presented in subsequent section.

$$\sigma_p = A\varepsilon^B e^{-C\varepsilon}\dot{\varepsilon}^D e^{-ET} \tag{2}$$

where ε - strain, $\dot{\varepsilon}$ - strain rate, T - temperature in C°, A, B, C, D, E - coefficients. Similar metamodel was developed to calculate strain distribution through the thickness of the strip. Numerous FE simulations were performed for various parameter and it was found that following function describes strain distribution with good accuracy:

$$\varepsilon(y) = \frac{2}{\sqrt{3}} ln\left(\frac{h}{h_1}\right)\left[1 + 3\left(\frac{0.387y\Delta}{y_{max}}\right)^2\right] \tag{3}$$

where: h_1, h - entry and current thickness of the strip, respectively, y coordinate through the thickness ($y = 0$ in the center and $y = y_{max} = h/2$ at the surface). Equation (3) allows to calculate strain at each location along the roll gap and through the thickness of the strip. Equation (1) allows further to calculate rolling torque (M_r) as well as electric current (I) and power (P) of the motor:

$$M_r = \psi F l_d \tag{4}$$

$$M_b = 2\mu_b F R_b \tag{5}$$

$$M_M = \frac{M_w + M_b + M_{bj}}{\eta_T \eta_M i} \tag{6}$$

$$P = M_s \omega \tag{7}$$

where: ψ - lever arm of the torque according to (Roberts 1983), i - transmission ratio, M_b - friction torque in bearings, M_N - nominal torque of the motor, M_{bj} - idle torque assumed as equal to $0.05M_N$, R_b - radius of the bearing, μ_b - friction

coefficient in the bearing, η_T, η_M - current and nominal angular velocity of the motor.

The equations describing components of the total torque were taken from [8]. The electric current of the motor was calculated from the electric power, depending on the type of the motor. For alternative current motors it was:

$$I = \frac{P}{U\cos(\varphi)} \tag{8}$$

where: U - voltage, φ - phase angle between voltage and current.

The equations presented in this section are used in the system to calculate all mechanical parameters as well as power and electric current required to run the rolling mill. These equations are coupled with thermal and microstructural models.

Thermal and Microstructural Models.
One dimensional solution of the Fourier equation was used to calculated temperature distribution through the thickness:

$$\frac{\partial}{\partial x}\lambda\frac{\partial T}{\partial x} + Q = \rho c_p \frac{\partial T}{\partial t} \tag{9}$$

where: T - temperature, λ - conductivity, x - coordinate along the thickness, ρ - density, c_p - specific heat, t - time.

Equation 9 has to satisfy the boundary condition on the top and bottom surface:

$$\lambda\frac{\partial T}{\partial x} = \alpha(T - T_a) \tag{10}$$

where: T_a - ambient temperature, α - heat transfer coefficient selected according to the current location of the strip.

Microstructure evolution model was based on works of Sellars (Sellars 1979). This model includes equations describing recrystallization and grain growth. The model is executed depending on strain and recrystallized material fraction according to the diagram presented in Figure 3. The diagram contains general approach for the austenite microstructure evolution simulation during the hot rolling process.

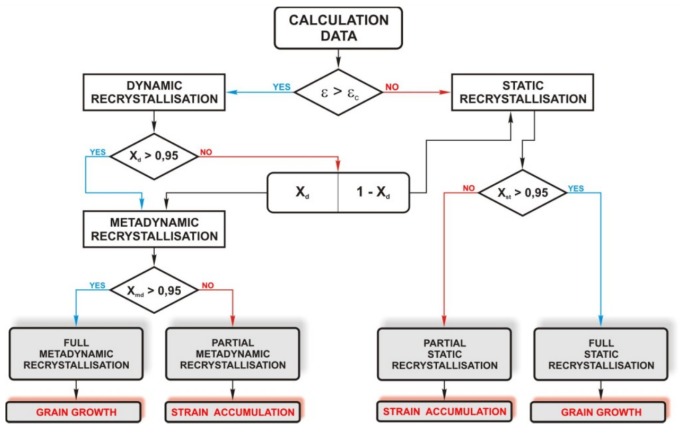

Figure 3: Flow of Calculations in Simulations of Microstructure Evolution (SRX, DRX and MTDRX Static, Dynamic and Metadynamic Recrystallization, respectively)

Prediction of the kinetics of phase transformations and volume fractions of phases after cooling was the main task of the laminar cooling model. Modified Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation was used to reach this task. The basic form of this equation is:

$$X = 1 - e^{-kt^n} \tag{11}$$

where: X - volume fraction of a new phase, k, n - coefficients, t - time. Modification of equation 11 included introduction of the coefficient k as a function of the temperature. Various functions $k = f(T)$ were used for different transformations (Pietrzyk and Kuziak 2012).

Coefficients in microstructure evolution equations for each steel in the database of the system were determined on the basis of stress relaxation tests or 2-step compression tests. Equations of the microstructural model with the description of coefficients for investigated steels are given in (Kuziak and Pietrzyk 2011). 1D thermal model allows to obtain very fast and reliable calculations, which do not require parallelization. On the other hand, microscale models are attached to selected integration points in hierarchical semi- or fully coupled way. Such implementation offers very flexible way of distribution of calculations onto HPC infrastructures, as well as facilitates collection of results. The algorithms used in microscale can be designed and implemented on the basis of different approaches, depending on the needs. This gives another possibility of distribution on the level of multicore computing devices e.g. GPGPUs or dedicated co-processors. Additionally, the computational module contains two numerical libraries: i) optimization library dedicated to determine optimal parameters for rolling mill devices; ii) sensitivity analysis library allowing investigation of particular parameters influence on final properties of the product.

EXPERIMENTAL EVALUATION

Rolling Mill Design

The created system was validated for typical configuration of the hot rolling line consisting of furnace, descaler, roughing mill, finishing mills, laminar cooling and coiler. The configuration of the most important parameters of particular devices is given in Table 1. The material model and its parameters are given in Table 2.

Table 1: Configuration Parameters of Devices

Device	Parameter	Value
Furnace	Temperature	1250 C°
	Slab width	1.5 m
	Slab length	11 m
	Slab thickness	0.22 m
Descaler	Pressure	180MPa
	Distance	0.3m
Roughing	Reversing mill with 5 passes	0.183, 0.141, 0.099, 0.058, 0.034 m
	Linear velocities	1.5, 1.8, 2.4, 3.0, 5.0 m/s
Finishing	6 two-high roll stands	0.023, 0.014, 0.0094, 0.0067, 0.0049, 0.004 m
	Linear velocities	1.17, 1.94, 2.97, 4.28, 5.88, 7.23 m/s
Laminar cooling	8 long sections divided into 2 subsections	Intensive cooling (1st subsection) = 30 m Normal cooling (1st subsection) = 30 m Intensive cooling (2nd subsection) = 40 Normal cooling (2nd subsection) = 20 m
Coiler	Distance from laminar cooling	80 m

Table 2: Material Models and their Parameters

Parameter	Value
Chemical composition	"Mn": 0.7, "C": 0.16, "Si": 0.03, "Nb": 0.01
Rheological model: Hensel-Spittel	"A": 2481.1, "B": 0.083937, "C": 0.1, "D": 0.12065, "E": 2.9803
Phase logic params	"Ca1": 0.0349, "Ca2": -0.0000403, "Cga1": 4.57, "Cga2": -0.005412, "Cgb1": -0.94, "Cgb2": 0.00228

For the evaluation purpose, we designed two data farming experiments. The input parameter set for both experiments contained the pressure parameter in 3 out of 8 devices performing laminar cooling. The parametrized devices were selected based on their more important role in the process. The pressure parameter is a float number with minimum value of 0 and maximum value of 100. The factorial design with 6 values for each pressure parameter was used. As the result each data farming experiment consisted of 216 distinct simulation runs.

HPC Infrastructure

We used two TOP500 clusters (Prometheus with peak performance of 2.4 PFlop/s and Zeus with peak performance of 374 TFlop/s) available at the Academic Computer Center Cyfronet AGH as our testbed. Prometheus includes Intel Haswell cores and NVidia K40XL GPU, while Zeus consists of Intel/AMD cores supported by NVidia M2050/M2090 GPU. Computing jobs simulating the metallurgical process were scheduled to both clusters through the Scalarm platform. Each scheduled job on Prometheus had been configured to use 24 cores, and each job scheduled on Zeus had been configured to use 12 cores. In both cases we scheduled 25 jobs on each cluster for the demonstration purpose.

Results

The collected results from the conducted evaluation can be split into two groups: domain-specific results and execution-related metrics.

The first group of results, domain-specific, includes information how the temperature of the rolling strips was changing in different places throughout the simulated metallurgical process. An example of such changes from a single simulation run is presented in Figure 4. Due to asymmetric nature of the results the temperature was measured at three points on the sample thickness: (1) axis, (2) middle and (3) surface.

Another domain-specific knowledge obtained from the simulations is information about volume fraction of phases with data collected on the surface part only. This information is essential to understand and predict the kinetics of phase transformations. Sample results are depicted in Figure 5.

In Table 3 the runtime metrics of simulation runs are collected from the experiments. The total experiment runtime includes runtime of all simulation runs including the queuing time. The executed numerical simulations are thread-based parallel applications. The observed runtime decrease is due to much higher cores-per-node density on Prometheus comparing to Zeus (24 to 12) and much more efficient cores themselves. However, the executed simulation is not linearly scalable between clusters. In addition, the queuing time was lower on

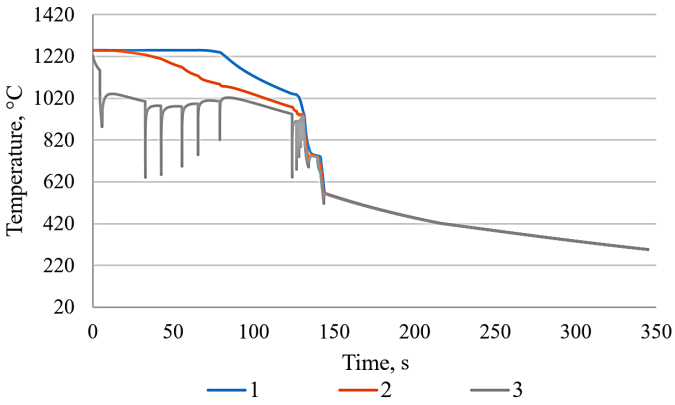

Figure 4: Temperature Change of the Simulated Steel Strips Throughout the Rolling Process (Measurement Points: 1 - Axis; 2 - Middle; 3 - Surface)

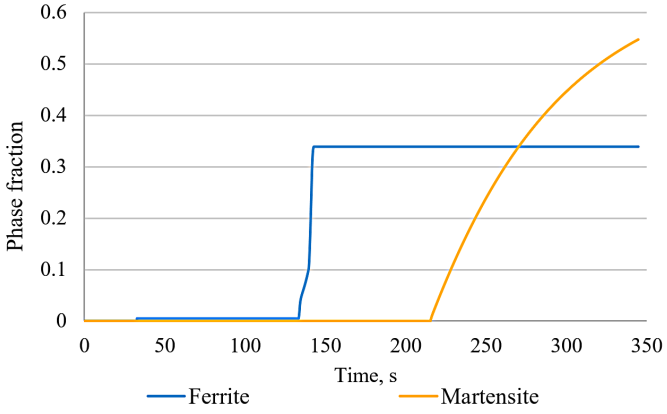

Figure 5: Simulated Volume Fractions of Phases

Premetheus, which is reflected by the total experiment runtime metric.

Table 3: Execution Time of Simulation

Cluster	Mean simulation runtime [min]	Total experiment runtime [min]
Zeus	53	606
Prometheus	38	392

CONCLUSIONS AND FUTURE WORK

In this paper we described the VirtRoll simulation system integrated with HPC clusters through the Scalarm platform for large-scale massive parallel computations. The system supports design of production technology of hot rolling strips. The main advantages of the VirtRoll system in comparison to other existing metallurgical systems is capability to study different numerical models, describing material behavior under loading conditions or during heat treatment. This allows to investigate the whole production process regarding aspects of data uncertainty and influence of different parameters of the models on final results of numerical simulations.

Detailed analysis of the results will be conducted in our future work. We plan to utilize data exploration techniques including sensitivity analysis and optimization methods, which can be

applied as the last step of the described experimental workflow. The main objective of this step is to develop better understanding of the hot rolling process and to discover pros and cons of the designed virtual rolling mill in terms of thermo-mechanical properties of the final products. In this context, data farming experiments will be used to provide large enough volume of data to perform a meaningful sensitivity analysis in order to reveal hidden relationships between simulation input and output.

ACKNOWLEDGEMENTS

Financial support of the Research Fund for Coal and Steel (RFCS), project no. RFSR-CT- 2013-00007, is acknowledged.

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