COLLISION MODELLING FOR HIGH ENERGY BALL MILLS USING EVENT DRIVEN SIMULATION

Roland Reichardt, Stephan Adam and Wolfgang Wiechert
Department of Simulation, Faculty 11/12, University of Siegen,
Paul-Bonatz-Str. 9-11, 57068 Siegen, Germany
{Reichardt, Adam, Wiechert}@simtec.mb.uni-siegen.de

ABSTRACT

Mills in general are used for grinding processes. This field of mechanical process engineering is dominated by empirical equations, caused by the difficulty of measuring the motion of the grinding media. In this paper, a high energy ball mill is presented as the subject of event driven simulation algorithms. The main steps of the algorithm are described. In detail, the collision response model of the ball's collision is derived and the differences with respect to classical approaches are explained. In order to make the simulation as realistic as possible, the simulation uses experimental values, measured with real material pairings. High speed videos of a transparent grinding chamber have been analyzed and compared to the simulation's visualisation in order to figure out the relevant parameters of the collision response model, which are essential. Simulation results and potential pitfalls of these kinds of simulations are discussed. It can be shown that the assumption that rotation of the balls and tangential forces are absent is an oversimplification.

INTRODUCTION

In materials engineering, high energy ball mills are used to develop new powder materials. The grinding medium, about 4000 steel balls in a lab scale mill, is accelerated by rotor blades in a horizontal drum (Fig. 1). Up to the present, only the overall energy balance has been measured experimentally (Zoz and Reichardt 1999). More substantial information such as, for example, the impact velocity distribution, still cannot be measured. Moreover, to understand the whole process, for example for the scale up from lab scale to industrial scale, it would be important to achieve a good understanding of the dynamics of the mill. As a matter of fact, up to now, the configuration of the process parameters has been carried out empirically.

From a simulatienst's viewpoint, ball mills are, mechanically, many body systems that are usually simulated by time continuous algorithms such as the discrete element approach.

Event driven algorithms - even though they are known to be far more efficient - have not become as popular. Event driven molecular dynamics simulations have been successfully applied to typical physical topics such as granular gases (Gavrilova et al. 2002, Reichardt and Wiechert 2003).

The basic concept of a discrete event simulation is presented in the following section. After this, the collision model is explained in detail. Furthermore different simulation experiments applying the different collision models are presented.

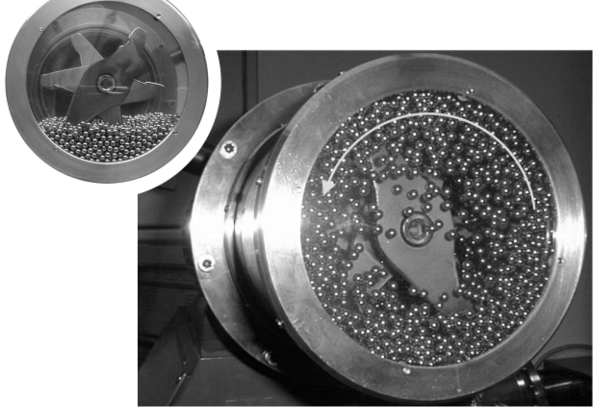

Figure 1: Operational mill; experimental transparent grinding chamber.

DISCRETE EVENTS

In this work, the high energy ball mill is described by an event driven particle simulation using collisions as basic events. The balls behave like dilute granular systems, where the mean free path of inelastically colliding particles is much larger than the average particle size. Furthermore, it is assumed that the balls do not build clusters of balls, in other words, that there are no multiple contact points, but rather only binary collisions (Brilliantov and Pöschel 2004). Pairwise collisions have been observed at typical rotor velocities for the grinding process. Of course, at low rotor speeds, the assumption of pairwise collisions becomes false, but the start phase of the milling process is very short in comparison to the total milling time. During the flight, it is assumed the there is no energy dissipation due to air resistance. In fact the milling chamber is evacuated.

Event List

Event driven molecular dynamics processes in general are modelled as a series of discrete instantaneous collisions. These events are stored in an event list ordered by time. Event lists are first mentioned in the late fifties of the last century (Alder and Winwright, 1959) and are still topics of research activities (Dahl et al. 2001, Miller and Luding 2004)

Generally, the event processing is an iteration over the steps 1-4 below:

Proceedings 19th European Conference on Modelling and Simulation
Yuri Merkuryev, Richard Zobel, Eugène Kerckhoffs © ECMS, 2005
ISBN 1-84233-112-4 (Set) / ISBN 1-84233-113-2 (CD)

1. The simulation clock jumps from one collision event to the next. The simulation time is updated by handling the next event of the event list, e.g. a ball to ball collision
2. The algorithm searches for the next possible collision time for each of the two balls involved. This is computed analytically. In a system of hard spheres, events refer to collisions, involving:
   - exactly two balls
   - one ball and the cylindrical walls of the drum
   - one ball and the flat side walls of the drum
   - one ball and one of the rotor blades

   The collision time is the flight time from the actual event to the new event.
3. The locations of the two new collisions are calculated using the flight time just computed to the collision point. The calculation of the collision response leads to the new flight direction at this point caused by the collision event.
4. These new events are inserted into the event list. Hereby, already predicted collisions may become invalid as a result of another ball crossing its flight path. In this case, the event list handling routine must ensure consistence by deleting the invalid event, and all events following.

The interested reader is referred to a previous publication with a more detailed description of this procedure (Reichardt and Wiechert 2003).

Collision Detection

In time continuous simulations, collisions are detected by object penetration checks after each time step. Contrary to this, in discrete event simulations, the collision detection (collision time) is computed analytically. The collision time is found when the distance function of two objects is zero for the first time. Mathematically speaking, the value sought is the minimum positive root of the distance over time. Taking into account the knowledge of physically impossible situations, the collision time of two balls can be calculated directly without case differentiation (Reichardt and Wiechert 2003). With regard to the ball to rotor collision, finding the first positive real root is more difficult (caused by the transcendental equation for the distance function).
Because the algorithm will observe only pairs of objects, ignoring the presence of the others, several collision times can be found. The minimum of these collision times is the only valid collision time, because this collision will occur first.
The efficient handling of the event list is a substantial task for discrete event simulation. New approaches for data structures and improvements of the algorithm have been presented in earlier publications (Marin et al. 1993, Reichardt and Wiechert 2003). The current implementation is able to calculate about 17000 collisions per second for 5000 balls, in other words; the calculation time is about 6 to 7 minutes for 1 second of real time.

COLLISION RESPONSE

The collision response model is fundamental to the accurate representation of a hard sphere simulation. Because the collisions are modelled to be instantaneous, the change in the flight direction and the energy dissipation during the collision are modelled to have zero duration. Mathematical equations which describe the collision response are the topic of recent theoretical investigations (Brilliantov and Pöschel 2004), but, to date, most of the equations implemented are oversimplified, as shown later.

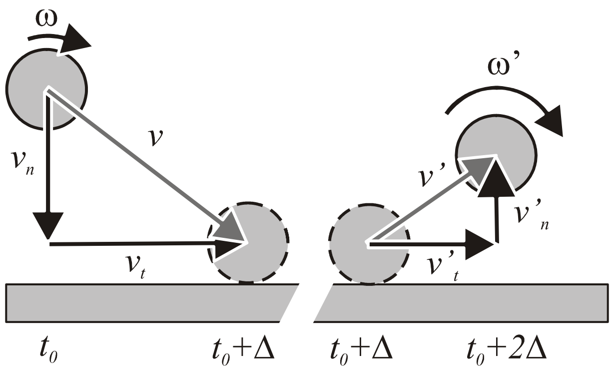

Figure 2: Velocity components of a ball before the collision (left) and after the collision (right).

The velocity of a ball is given by the velocity vector, v, which can be divided into its component in the normal direction, v_n, and in the tangential direction, v_t. Furthermore, the ball's initial rotation is given by the rotational vector, ω. The direction of ω can be understood as the rotational axis of the ball; the magnitude of ω is the rotational speed. The desired values are the velocity vector, v', and the rotational vector, ω', just after the collision. Figure 2 illustrates the situation described.

Normal Coefficient of Restitution

Energy will be dissipated during collision, which results in a lower kinetic energy after the collision. The ratio of the (relative) velocity in the normal direction before and after the collision is the normal restitution coefficient, ε_n. A fully elastic collision, without any energy dissipation, is represented by $\varepsilon_n = 1$, whereas a fully plastic collision is represented by $\varepsilon_n = 0$. Physically, the loss of kinetic energy in the normal direction will cause the ball to bounce back at a lower angle.

$$\vec{v}_n{}' = -\varepsilon_n \vec{v}_n \qquad (0 \le \varepsilon_n \le 1) \qquad (1)$$

Even if, in equation (1), ε_n appears to be a constant, in reality it is velocity dependent. By dimensional analysis it was first proven that a constant coefficient of restitution is not consistent with physical reality (Tanaka et al. 1991). Later, this fact was proven analytically (Brilliantov et al. 1996). Unfortunately, the theoretical equations require additional experimental investigations to assign values to the material dependent parameters.

Usually, energy dissipation caused by collisions is modelled to be velocity independent, whereas in reality it increases at higher velocities. In order to make the simulation as realistic as possible, an experimental setup has been designed and constructed to measure the velocity dependent energy dissipation during the collision of objects. The collision zone has been observed by a high speed video camera. The resulting sensor data were analyzed by image processing, which recognizes the balls within each frame of the movie. Using these coordinates, the velocity just before and just after the collision can be calculated – their quotient is the desired value (restitution coefficient). In a prior project, an experimental setup has been designed to measure the restitution coefficient in the normal direction of ball bearing spheres and a stainless steel plane. The material pairings are exactly those of the real mill. The velocity dependent restitution coefficient shown in Figure 3 has been measured.

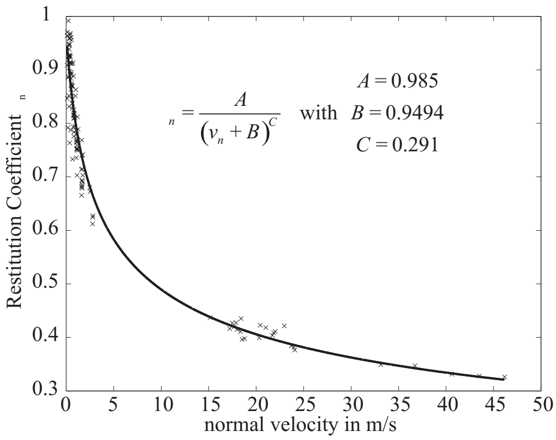

Figure 3: The velocity dependent restitution coefficient in the normal direction.

The simulation results presented in this paper are calculated using both constant and velocity dependent restitution coefficients.

The collision response of two balls with the same mass can be calculated using equation (2). Here, $\vec{e}$ is the unit vector through the balls' centres during the collision.

$$\vec{v}' = \vec{v} \pm \frac{1}{2}(\varepsilon_n + 1)(\vec{v}_{rel}\,\vec{e})\,\vec{e} \tag{2}$$

Tangential Coefficient of Restitution

By introducing rotation, it is not the velocity components of the centres of mass that are important, but rather the velocity of the surfaces of the balls at the point of contact in the normal and in the tangential direction. This is, for identical balls with the same mass and the radius R,:

$$\begin{aligned} \vec{g}_n &= (\vec{v}_{rel}\,\vec{e})\,\vec{e} \\ \vec{g}_t &= \vec{v}_{rel} - \vec{g}_n + R\left(\vec{e} \times \left(\vec{\omega}_1 + \vec{\omega}_2\right)\right) \end{aligned} \tag{3}$$

Note that $\vec{g}_n$ is simply the relative velocity in the normal direction, whereas $\vec{g}_t$ is the relative velocity in the tangential direction and, additionally, the velocity of the surfaces caused by the rotation of the balls.

To describe the change of the tangential component of the (relative) velocity, the coefficient of tangential restitution has to be introduced. Rotation of the balls contributes to the tangential component of their relative motion at contact. Hence, the balls' collision response is completely described by two coefficients of restitution:

$$\begin{aligned} \vec{g}_n{}' &= -\varepsilon_n \vec{g}_n \qquad (0 \le \varepsilon_n \le 1) \\ \vec{g}_t{}' &= \varepsilon_t \vec{g}_t \qquad (-1 \le \varepsilon_t \le 1) \end{aligned} \tag{4}$$

This yields two velocities after the collision:

$$\vec{v}' = \vec{v} \pm \frac{1}{2}\left(\left(\varepsilon_n + 1\right)\vec{g}_n + \left(1 - \varepsilon_t\right)\vec{g}_t\right) \tag{5}$$

For the frictionless case, $\varepsilon_t = 1$, equation (5) is reduced to equation (2). In reality, during a collision, the normal force is not a constant. It increases from zero at the beginning of the collision to the moment of maximum compression, and decreases during the rest of the collision. Therefore, the tangential type of contact, sliding and rolling, may change during the impact. The complicated dynamics of such collisions is known (Stronge 1990).

Simplified, the collision time is assumed to be zero, and, therefore, the tangential restitution coefficient accounts for the energy dissipation of the collision. Note that, due to the discrete event approach, collision durations are not permitted. Further, it is assumed that the loss of kinetic energy in the tangential direction is equal to the increase of rotation per ball:

$$\vec{\omega}' = \vec{\omega} + \frac{\left(1 - \varepsilon_t\right)\left(\vec{e} \times \vec{g}_t\right)}{2R} \tag{6}$$

Hence, energy is dissipated in the normal direction only, not in the tangential direction.

It should be noted that the tangential velocity component is reduced by the tangential restitution coefficient. Therefore, the ball is pushed away from a wall because the response angle is increased at the moment of bounce.

SIMULATION EXPERIMENTS

Distributed simulations have been performed using 256 processor computer clusters. Without applying the discrete event algorithm, these experiments could not been concluded within a reasonable time. We have conducted variation studies of velocity dependent and velocity independent restitution coefficients. Furthermore, we have carried out parametric studies to show the influence of the tangential restitution coefficient, and thus the influence of the balls' rotation.

Initially, the balls are equally distributed in space and the directions of the velocity vectors are also equally

distributed. The magnitude of the velocity vector – the absolute velocity – has been set to one meter per second for all balls. When setting up the initial conditions, the algorithm will guarantee that there are no object penetrations. Of course, this setup is not realistic. Therefore, the simulation has to run until the initial setup no longer influences the simulation results. This is measured by observing the histogram of the absolute velocities of the balls, which are represented by their median.
These histograms are generated every 0.03 seconds of simulated time, which has been shown to be a reasonable time interval. As well as the histogram of the absolute values, several other histograms are generated during simulation time, e.g. the histogram of the impact velocities in the normal direction, which are important for the understanding of the milling efficiency. In this paper, the focus is set on the median of the absolute velocity as a representative value.

Steady State of the Simulation

The steady state of the simulation is reached when the simulation has "forgotten" its initial setup. From this point on, the median of the absolute velocity has reached an asymptotic value, which will not change significantly with increasing simulation time. The median values are smoothed by a median filter over the past three measurement points.

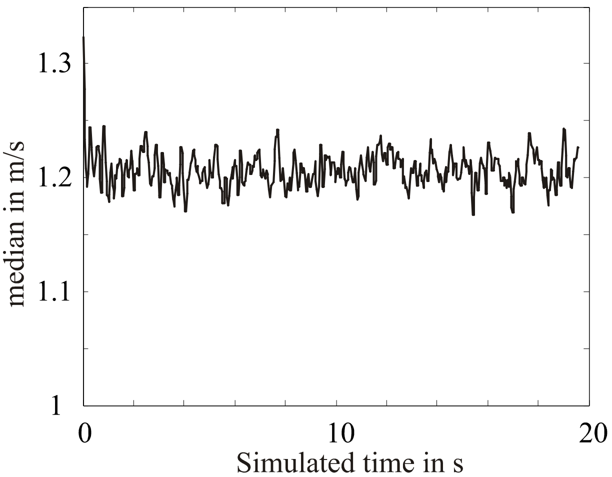

Figure 4: Representative progression of a median over simulation time.

The asymptotic behaviour of the median of a typical simulation is shown in Figure (4). Although shown indirectly by the y-axis scale, the range is between 1.0 – the initial setup of the simulation – and above 1.35, which is caused by the initial impulse of the rotor blades. A stationary behaviour is observed beyond 0.5 seconds of simulation time. Nevertheless, every simulation has been calculated for 30 seconds, even if this is not shown in every figure.
The simulations have been visualised and animated using the ray tracer software program POWRAY 3.6 (Fig. 6). The scripts for these animations are generated by the simulation software.

RESULTS

Constant Restitution Coefficient

As assumed in most simulations of this type, the rotational influence is ignored and the normal restitution has been assumed to be constant, even though this has already been explained previously to be false. Various simulations with this approach have been performed for a range of $\varepsilon_n = 0.75 \ldots 0.95$, which is a popular range in the literature for arbitrary kinds of material pairings.

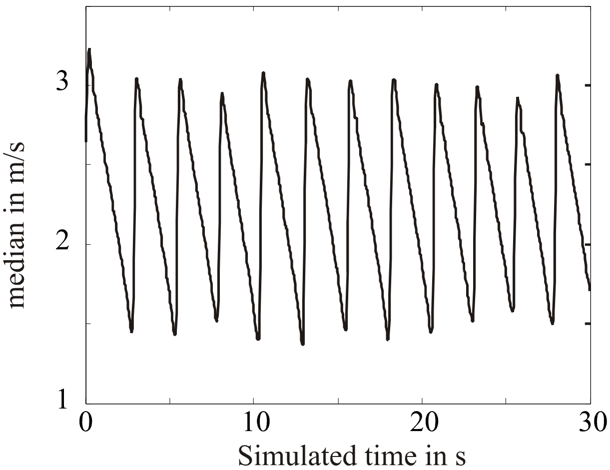

Figure 5: Simulation with constant restitution coefficient. The saw tooth curve is not realistic.

Surprisingly, a synchronising effect was observed. Just after the start of the simulation, the balls are pushed by the rotor blades towards the inner surface of the grinding chamber and then "roll"- this is not really possible in discrete event simulations – along the surface, where their velocity is decreasing to a certain threshold (Zoz et al. 2002). This critical velocity is reached when the gradient of the parabolic flight path is lower then the gradient of the cylindrical grinding chamber. After this, they fall in a parabolic flight path into the grinding chamber.

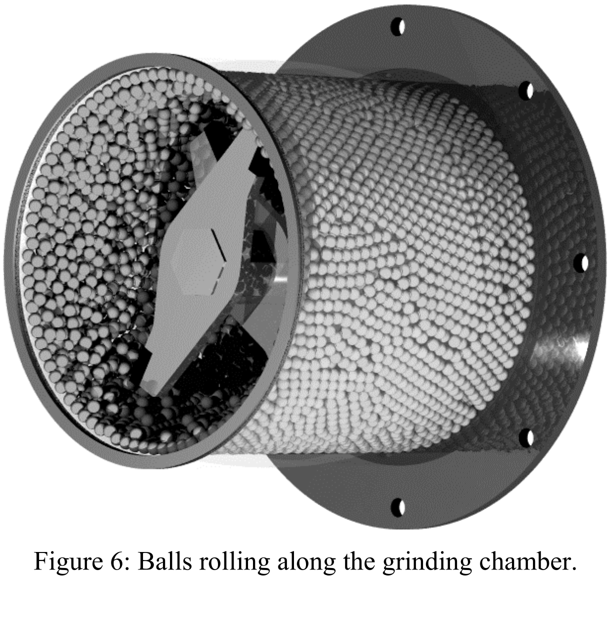

Figure 6: Balls rolling along the grinding chamber.

At every collision with the wall, the ball's trajectory moves closer to the wall, as explained earlier. Hence, all balls move along the inner surface of the grinding chamber. In the outer regions of the grinding chamber, the balls are no longer within the reach of the rotor blades, as there is a distance of three ball diameters between the rotor tips and the inner surface.
Due to their tangential trajectories, only ball to ball collisions reduce their speed. As a consequence of the high ball density in the outer regions, the balls synchronise their speed – see Figure 6. This behaviour can be observed at all relevant rotational speeds.
Summarizing, it can be said that, as well the high ball density at the outer regions of the grinding chamber, the periodic accelerations are not realistic. Hence, the collision response model used in these simulations is oversimplified.

Velocity dependent Restitution

The first improvement to the classical damping model is the implementation of the velocity dependent restitution coefficient based on the measured values of Figure 3. This leads to high energy loss at high relative velocities, e.g. at the rotor collisions, and to low energy loss at low relative velocities in the normal direction, e.g. the bouncing of a ball along the inner surface of the grinding chamber. Varying the rotor speed results in a narrower spectrum of velocity distributions. Even if the motion is more realistic, the balls are still located at the outer regions of the grinding chamber, which is not realistic.

Including tangential Restitution

As demonstrated by the previous experiments, the classical collision response model must be changed to achieve more realistic results. This is achieved by considering the rotation of the balls and the tangential restitution coefficient.

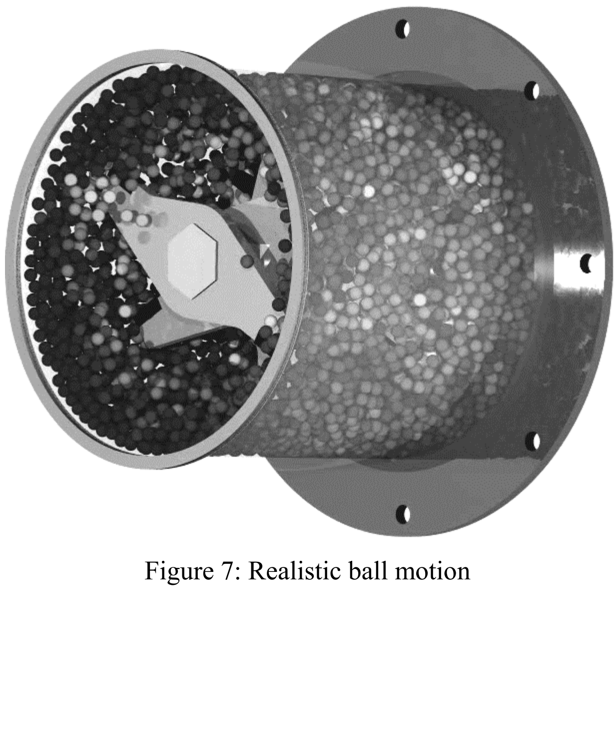

Figure 7: Realistic ball motion

The collision response model of the simulation has been expanded to take into account the dynamic normal restitution coefficient and a constant tangential restitution coefficient.
The analysis of the median values – see Figure 4 – has shown an asymptotic behavior, as in the real mill. Observations of the simulation visualizations have confirmed this realistic ball motion, because the balls' trajectories are very similar to those observed by the high speed video camera – see Figure 1. Consequently, the simulation using both restitution coefficients is able to reproduce the grinding media's motion.
In addition to the higher degree of realistic representation of these simulations, the CPU time has been reduced. This is caused by the more infrequent, but more realistic, collisions. The "rolling" effect of the prior set of simulation described in the previous section implies collisions with a very short distance, and, therefore, is time consuming.
In the current configuration, the simulation calculates approximately 6 minutes for 1 second of simulated time, including the generation of the various histograms

CONCLUSION

In this paper, we present a new application for discrete event simulation, namely, a high energy ball mill. A brief description of the algorithm using collision events as discretization markers, and the explanation of the analytical collision detection algorithm has been given. In detail, the collision response model has been explained. It has been shown that the energy lost during a collision can be described by two parameters, the tangential and normal restitution coefficients.
In two simulation experiments, the influence of the collision response model on the validity of the simulation has been shown. The classical simplified approach to calculate the collision response using solely a constant restitution coefficient in the normal direction has been shown to be an oversimplification. In a second experiment, we have implemented a velocity dependent restitution coefficient in the normal direction, and a constant restitution coefficient in the tangential direction. This approach leads to realistic ball motion inside the mill. The advantage of this simulation technique, namely the high efficiency, has been demonstrated.

OUTLOOK

In future work, the collision response model has to be expanded by implementing a velocity dependent tangential restitution coefficient. Unfortunately, significant experimental efforts have to be expended to measure these values. Nevertheless, this simulation is able to reproduce the balls' motion. Hence, it can be used to assist design engineers to optimize rotor blades or the shape of the grinding chamber. Furthermore, it can be used to calculate the motor's energy consumption based on the milling chamber's geometry.

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AUTHOR BIOGRAPHIES

ROLAND REICHARDT studied mechanical engineering at the University of Siegen, Germany. He worked from 1997 to 2001 for a mechanical process engineering company of mills of varying type, initially as the head of software department, and, later, in the company management. In 2002, he returned to the University of Siegen, where he is now a scientific assistant at the Chair of Simulation and Computer Science. Currently, he is working on his doctoral thesis.

WOLFGANG WIECHERT studied mathematics and computer science at the University of Bonn and obtained his diploma degree in 1985. Subsequently, he joined the Department of Theoretical Biology at the University of Bonn, where he obtained his PhD in 1991. From 1991 to 1996, he worked in the Institute of Biotechnology at the Jülich Research Center, where he earned his postdoctoral lecturer’s qualification. Since 1996, he has been professor for simulation at the Institute of Systems Engineering at the University of Siegen.