WIAS

Weierstrass Institute for Applied Analysis and Stochastics

Leibniz Gemeinschaft

FORSCHUNGSverbund Berlin e.V.

"Intelligent solutions for complex problems"

Annual Research Report 2005

Cover figure: Calculation of a stress- and temperature-induced morphology on the µm scale of a tin-lead solder joint

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Prof. Dr. Jürgen Sprekels, Director

The Weierstrass Institute for Applied Analysis and Stochastics (WIAS, member of the Leibniz Association) presents its Annual Report in its new design for the first time. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2005. Following a more general introduction in part one, in its second part seven selected scientific contributions, written for a broader public, highlight some results of outstanding importance. Finally, the third part presents the essential results of the research groups.

In contrast to the previous two years, which were marked by the very successful external evaluation of WIAS by the Senate of the Leibniz Association and by structural changes, 2005 has been a "normal" year. Scientifically, it has again been successful. The work in the *Research Program 2004–2006* is in good progress, and despite funding cuts and increasing competition, WIAS has consolidated its leading position in the mathematical community as a center of excellence in the treatment of complex applied problems. Several scientific breakthroughs were achieved, some of which will be detailed later in this report, and WIAS has even expanded its scope into new applied problems from medicine, economy, science, and engineering, especially in its main fields of competence:

- Nano-, and optoelectronics
- Optimization and control of technological processes
- Phase transitions and multifunctional materials
- Stochastics in science and economics
- Flow and transport processes in continua
- Numerical methods of analysis and stochastics

The positive development is reflected by an increased acquisition of grants, by the number of international workshops organized by the institute, by numerous invited lectures held by WIAS members at international meetings and research institutions, and by the many renowned foreign visitors hosted by the institute last year.

The number of refereed journal publications was the same as in 2004. In addition to this, no less than five excellent monographs authored by WIAS members appeared in renowned scientific series of top-selling publishing companies. Each one of these monographs marks a milestone and culmination point of long-standing research at WIAS, and is visible evidence for the scientific excellence of its collaborators. As a special highlight, Dr. John Schoenmakers's book *Robust Libor Modelling and Pricing of Derivative Products* was chosen by RISKBOOK.com into the "Top Ten Finance Books" of 2005.

As another highlight of 2005, Prof. Anton Bovier, the second Deputy Director of WIAS, was invited to deliver a lecture at the International Congress of Mathematicians 2006 in Madrid; he will be one of only eight German speakers at this World Congress.

The high rank of WIAS in the mathematical community is also witnessed by the fact that the year-long success story of "Transfer of knowledge via brains" through the institute's members continued also in 2005: Dr. Markus Reiß was appointed W3 Professor for Statistics at the University of

Heidelberg. Since the institute's foundation in 1992, a total of 31 calls (including 16 to full professorships in Germany and nine to professorships abroad) have been received by WIAS members; given the fact that presently there are 54 scientists on the budget of WIAS, this is a truly remarkable output of which we are proud.

2005 has also been a "year of workshops" at WIAS. No less than 12 international workshops organized by WIAS, the largest number ever, evidenced the institute's reputation and its role as an attractive meeting place for international scientific exchange and cooperation. In addition to this, WIAS members (co-) organized numerous scientific meetings throughout the world; in particular, the WIAS Director Prof. Jürgen Sprekels was one of the organizers of a meeting at the Mathematisches Forschungsinstitut Oberwolfach (MFO).

One of the workshops held at WIAS, the MATHEON Workshop "Mathematics in Industry: Process Engineering of Thin Liquid Films" co-organized by the WIAS member PD Dr. Barbara Wagner, deserves special recognition, since it followed a novel concept. On the first day of this workshop, representatives from industry introduced concrete industrial problems; these were tackled by small interdisciplinary teams that during the following two days developed mathematical models and solution ideas. On the final day of the workshop, the results obtained by the teams have then been presented to the industrial partners. This workshop concept turned out to be a very promising line of approach toward the mathematical treatment of problems from industry.

The year 2005 was also marked by the introduction of the "WIAS Postdoctoral Fellowships". These fellowships, which are granted for visits at WIAS for up to one year, give their holders the opportunity to participate in the applied research projects of WIAS. We are hoping that this new instrument of international exchange and cooperation will attract outstanding junior researchers from all over the world.

In addition to these "global" activities, WIAS has on the "local" scale intensified its well-established cooperation with the other mathematical institutions in Berlin, with the main attention directed toward the three Berlin universities. This is witnessed by the fact that as of today five leading members of WIAS, including the director and his two deputies, hold special chairs funded by WIAS at the Berlin universities. Another such appointment is under way, and we are hoping that by the end of 2006 six WIAS members will hold chairs funded by WIAS at the Berlin universities.

Besides these activities, and besides the cooperation with the universities through the manifold teaching activities of its members, WIAS initiated and participated in successful applications for Collaborative Research Centers, Priority Programs, and Graduate Colleges of the German Science Foundation (DFG). For example, the institute contributes considerably to the DFG Graduate College "Analysis, Numerics, and Optimization of Multiphase Problems" at the Humboldt-Universität zu Berlin.

The highlight of cooperation with the mathematical institutions in Berlin, however, was also in 2005 the joint operation of the DFG Research Center MATHEON "Mathematics for key technologies" located at the Technical University of Berlin. Annually, DFG funds exceeding 5.5 million euros flow into Berlin for MATHEON to become an international beacon of applied mathematics. WIAS is committed to the success of the Center by providing considerable financial and personal resources:

the Director of WIAS is a member of MATHEON's Executive Board, both his deputies are "Scientists in Charge" of mathematical fields in the center, and members of WIAS participate in the management of 13 of its subprojects. In turn, in 2005 up to ten scientific collaborators and several student assistants employed at WIAS were funded by MATHEON. Presently, all efforts are directed towards winning a second funding period for MATHEON for the years 2006–2010.

Our primary aim remains unchanged: to join fundamental research with application-oriented research, and, by new scientific insights, to contribute to the advancement of innovative technologies. Owing to the continued effective reduction in our basic funding during the past years, it has become more and more difficult to meet all expectations; however, thus far WIAS has been able not only to keep up its scientific output on a high level, but even to increase it by an optimal use of its resources and its capacities.

But now a limit has been reached: A sufficient basic funding is imperative for the institute to maintain its success in the scientific competition, particularly for grants and industrial cooperation partners, but also for qualified collaborators. Therefore, the institute views with much concern the continuing erosion of its budget.

As in the past years, we hope that funding agencies, colleagues and partners from industry, economy, and sciences will find this report informative and will be encouraged to cooperate with us.

Berlin, in January 2006

J. Sprekels

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1 Presenting WIAS

- Profile
- Structure and Scientific Organization
- Grants

1.1 Profile

The *Weierstrass Institute for Applied Analysis and Stochastics* (Weierstraß-Institut für Angewandte Analysis und Stochastik, WIAS) is part of the *Forschungsverbund Berlin e.V. (FVB)*. FVB is a legal entity in which eight scientifically independent member institutes of the *Leibniz Association* are combined. The *Director of WIAS* is responsible for the scientific work at WIAS, the *Manager* of the *Common Administration of FVB* is in charge of its administrative business.

The mission of WIAS is to carry out *project-oriented* research in applied mathematics. WIAS contributes to the solution of complex economic, scientific, and technological problems of supraregional interest; its research is interdisciplinary and covers the entire process of problem solution, from modeling to the mathematical analysis of the models, to the development and implementation of efficient and robust algorithms, and the simulation of technological processes. In its field of competence, WIAS plays a leading role in Germany and worldwide.

WIAS promotes the international cooperation in applied mathematics by organizing workshops and running guest and postdoc programs. A special emphasis is devoted to the extension of the institute's traditional contacts to the scientific institutions of Eastern Europe.

A successful mathematical approach to complex applied problems necessitates a long-term multiply interdisciplinary cooperation in project teams. Besides maintaining the contact to the customers from the applications, which means, in particular, to master their respective technical terminologies, the WIAS members have to combine their different mathematical expertises and programming skills. This interdisciplinary teamwork takes full advantage of the possibilities provided in a research institute. It also advances the internal scientific networking and helps optimizing the common efforts of the institute's scientific staff.

1.2 Structure and Scientific Organization

1.2.1 Structure

To fulfill its mission, WIAS is presently structured in departments for technical services and the seven scientific research groups[1]

RG 1. Partial Differential Equations

RG 2. Laser Dynamics

RG 3. Numerical Mathematics and Scientific Computing

RG 4. Nonlinear Optimization and Inverse Problems

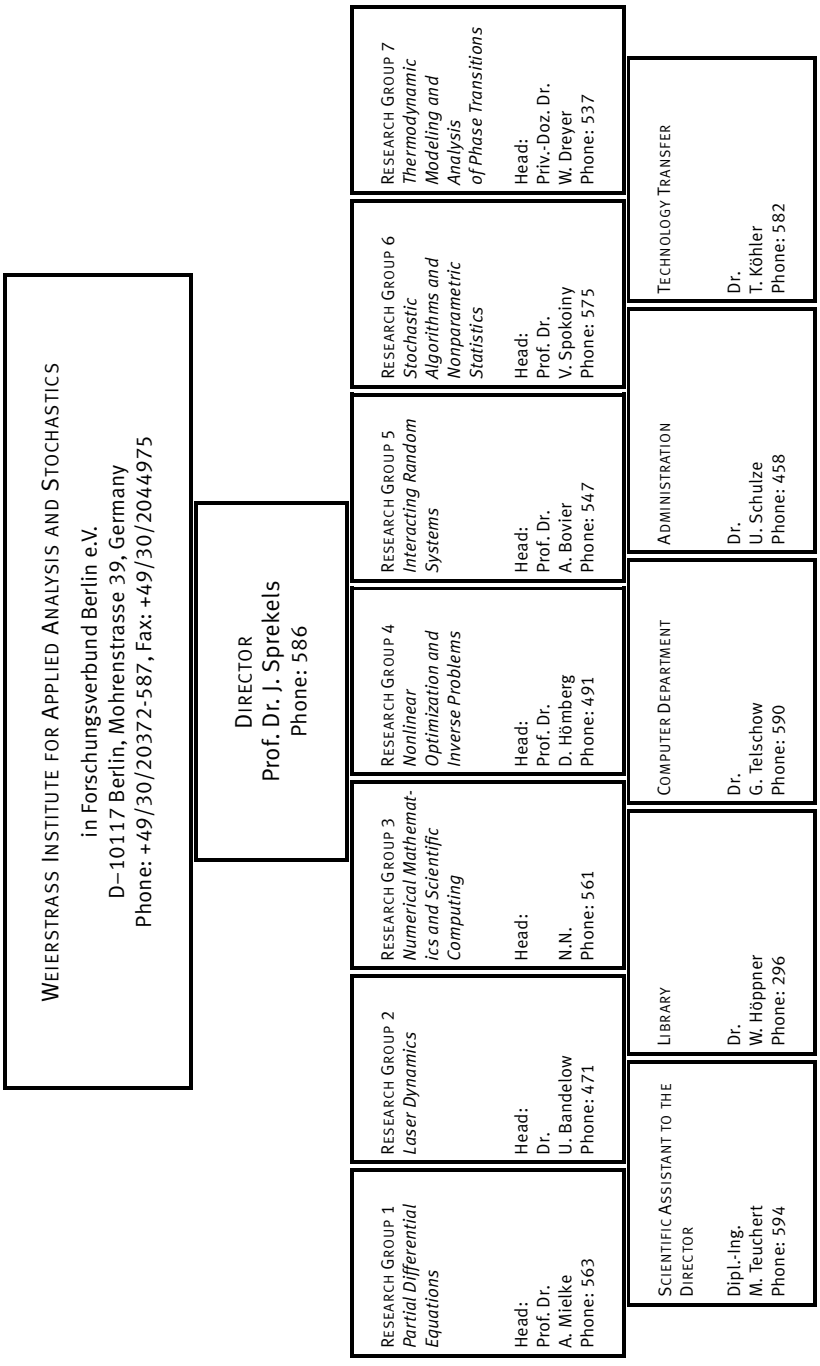
RG 5. Interacting Random Systems

RG 6. Stochastic Algorithms and Nonparametric Statistics

RG 7. Thermodynamic Modeling and Analysis of Phase Transitions

[1] In the following, the term "research group" will often be abbreviated by "RG".

The following organization chart gives an overview of the organizational structure:



1.2.2 Main Fields of Research

The research at WIAS is presently focusing on the following *main fields*, in which the institute has an outstanding competence in modeling, analysis, and simulation:

- **Nano- and optoelectronics**
- **Optimization and control of technological processes**
- **Phase transitions and multifunctional materials**
- **Stochastics in science and economics**
- **Flow and transport processes in continua**
- **Numerical methods of analysis and stochastics**

To these fields, WIAS has made important contributions in the past years that strongly influenced the directions of development of worldwide research. The institute has a special modeling and simulation expertise in two promising modern technologies:

- Optical technologies (in particular, diffractive and laser structures, optical fibers)
- Fuel cells (direct methanol fuel cells)

1.2.3 Contributions of the Research Groups of WIAS

The seven research groups form the institute's basis to fully bring to bear and develop scope and depth of its expertise. The mathematical problems studied by the research groups originate both from short-term requests arising during the solution process of real-world problems, and from the continuing necessity to acquire further mathematical competence as prerequisite to enter new fields of applications. This necessitates a well-directed long-term *basic research in mathematics*.

The following table gives an overview to which main fields the research groups have contributed in 2005 in the interdisciplinary solution process described above.

Main Fields	RG 1	RG 2	RG 3	RG 4	RG 5	RG 6	RG 7
Nano-, and optoelectronics	*	*	*	*	–	–	–
Optimization and control of technological processes	–	–	*	*	–	*	*
Phase transitions and multi-functional materials	*	–	*	*	*	–	*
Stochastics in science and economics	–	–	*	*	*	*	*
Flow and transport processes in continua	*	–	*	–	*	*	*
Numerical methods of analysis and stochastics	*	*	*	*	*	*	*

In the following, we list special research topics that have been addressed in 2005 within the general framework of the main fields. The research groups that have contributed to the respective studies are indicated in brackets.

1. Nano- and optoelectronics

- Technology and device simulation of semiconductor devices (in RG 1 and RG 3)
- Phenomenological modeling of semiconductor heterostructures (in RG 1)
- Diffractive optics (simulation and optimization of optical gratings; in RG 4)
- Quantum mechanical modeling of nanostructures (in RG 1)
- Laser structures (in RG 1 and RG 2)

2. Optimization and control of technological processes

- Simulation and control in process engineering (in RG 3 and RG 4)
- Virtual production planning (optimization and inverse modeling of multibody systems; in RG 3 and RG 4)
- Problems of Optimal Shape Design (in RG 4 and RG 7)
- Optimal control of heat treatments and milling processes (in RG 4 and RG 7)

3. Phase transitions and multifunctional materials

- Modeling of nonlinear phenomena and phase transitions in multifunctional materials (hysteresis in shape memory alloys and piezo effects in ferromagnetic and ferroelectric materials; in RG 1 and RG 7)
- Thermomechanical modeling of phase transitions in steels (in RG 4 and RG 7)
- Modeling and simulation of gas–liquid and liquid–solid transitions, phase separation with thermomechanical diffusion (Stefan problems, phase field models, LSW theory, Becker–Döring models; in RG 7)
- Stochastic modeling of phase transitions (in RG 5)
- Growth of semiconductor bulk single crystals (silicon carbide, aluminum nitrite, gallium arsenide; in RG 7)

4. Stochastics in science and economics

- Stochastic particle systems and kinetic equations (modeling and simulation of coagulation processes and gas flows; in RG 5, RG 6, and RG 7)
- Modeling of stock prizes, interest rates, and exchange rates (in RG 5 and RG 6)
- Evaluation of derivatives, portfolio management and evaluation of risk (in RG 6)
- Nonparametric statistical methods (image processing, financial markets, econometrics; in RG 6)
- Dynamical processes in nonhomogeneous media (in RG 5 and RG 7)

5. Flow and transport processes in continua

- Treatment of Navier–Stokes equations (in RG 3 and RG 7)
- Flow and mass exchange in porous media (water and materials transport in soils and in porous rocks, two-phase flows; in RG 3)
- Modeling of fuel cells (in RG 3)
- Modeling of nanostructures of thin films on crystalline surfaces (in RG 7)

6. Numerical methods of analysis and stochastics

- Numerical solution of partial differential equations (finite volume and finite element methods, preconditioners, grid generation, error estimators, and adaptivity; in all research groups, especially in RG 3)
- Numerics of inverse problems (integral equations, regularization techniques; in RG 1, RG 4, and RG 6)
- Nonlinear optimization techniques (in RG 4)
- Stochastic numerics (Monte Carlo methods, kinetic equations, coagulation dynamics, particle systems; in RG 5, RG 6, and RG 7)
- Development of WIAS software packages (`AWS`, `BOP`, `ClusCorr98`, `DiPoG`, `gltools`, `LDSL-tool`, `pdelib2`, `TetGen`, `WIAS-HiTNIHS`, `WIAS-SHarP`, `WIAS-TeSCA`, `WIAS-KPLIB`, `WIAS-QW`)

1.3 Grants

The raising of grants under scientific competition is one of the main indicators of scientific excellence and thus plays an important role in the efforts of WIAS. In this task, WIAS has been quite successful in 2005, having increased the total sum from 1.30 million euros to 1.77 million euros, from which additional 25.75 researchers (Dec. 31, 2005) have been financed. Remarkable, and particularly welcome is the fact that in a time of low economical growth the funds raised in industrial collaborations could be increased to 296,000 euros. In total, 31.6 per cent of the total budget of WIAS in 2005, and 33.1 per cent of its scientific staff, originated from grants. In the following, some projects of particular interest and importance will be highlighted, without going into too much detail[2].

1.3.1 DFG Research Center MATHEON

The highlight of cooperation with the mathematical institutions in Berlin has been the joint operation of the DFG Research Center MATHEON “Mathematics for key technologies”. Annually, DFG

[2] For a detailed account of projects funded by third parties, we refer the reader to the appendix, Section A.2 Grants below.

funds exceeding 5.5 million euros flow into Berlin for MATHEON. WIAS dedicates considerable financial and personal resources to the Center: its director is a member of MATHEON's Executive Board, both his deputies are "Scientists in Charge" of mathematical fields in the Center, and members of WIAS participate in the management of 13 of its subprojects. In turn, in 2005 up to ten scientific collaborators and several student assistants at WIAS were funded by MATHEON.

Presently, the peer review process for a second funding period of MATHEON (June 1, 2006 – May 31, 2010) is under way. For this period, 14 projects headed by WIAS members have been selected by the Center in a highly competitive process. In case that a second funding period will be granted by DFG, a total of 12.5 additional researchers will be financed by MATHEON at WIAS.

1.3.2 DFG Graduate College GRK 1128 *Analysis, Numerics, and Optimization of Multiphase Problems*

In the Graduate College GRK 1128 at Humboldt-Universität zu Berlin, which started operations in April 2005 (first funding period: until September 2009), a number of WIAS members are active as principal investigators and associate members; Prof. D. Hömberg (RG 4) is its Deputy Coordinator. WIAS members are presently supervising the theses of three graduates.

1.3.3 DFG Priority Program SPP 1095 *Analysis, Modeling, and Simulation of Multiscale Problems*

This DFG program, which is in its final funding period and coordinated by the first Deputy Director of WIAS, Prof. A. Mielke, is now being administered by WIAS; in particular, the coordinator's funds will be managed by WIAS for the remainder of the funding period.

1.3.4 Krist$\widetilde{Mag}$

In this research project, which is being funded since July 2005 in the "Zukunftsfonds" of the state of Berlin and headed by the Institute of Crystal Growth in Berlin-Adlershof, WIAS cooperates with several industrial companies and other research institutions. The project aims at the development of a new technique for the crystal growth from a melt under the impact of magnetic fields.

1.3.5 BMBF Project *Numerical simulation for direct methanol micro fuel cells*

This research project, wich started operations in 2005 and will run until June 2008, is part of the nationwide network "H_2 and Methanol Polymer Electrolyte Fuel Cells" funded by BMBF. This network, which combines four smaller subnetworks, is chaired by the current head of RG 3, Dr. J. Fuhrmann.

1.3.6 International Graduate College *Stochastic Modeling of Complex Processes* of the DFG

This international graduate college, which shall be operated jointly with ETH Zürich and University of Zurich, Switzerland, has been applied for and is presently under review. In case that it will be granted by DFG, its first funding period will be July 2006 – December 2011. It will be located at the Technical University of Berlin, and its designated coordinator is Prof. A. Bovier, the second Deputy Director of WIAS.

2 Scientific Highlights

- Stochastic Models for the Boltzmann Equation
- Pulse Dynamics in Mode-locked Lasers for Optical Telecommunications
- Regularity for Elliptic and Parabolic Differential Equations
- Phase Transitions and the Evolution of Precipitates in Crystalline Solids
- Analysis and Numerics for Nonlocal Phase Separation Processes
- Spatially Adaptive Analysis of fMRI Experiments
- The Block Oriented Process Simulator BOP

2.1 Stochastic Models for the Boltzmann Equation

Wolfgang Wagner

Kinetic theory and applications

Fig. 1: *James Clerk Maxwell (1831–1879)*

Kinetic theory describes a gas as a system of many particles (molecules) moving around according to the laws of classical mechanics. Particles interact, changing their velocities through binary collisions. The gas is assumed to be sufficiently dilute so that interactions involving more than two particles can be neglected. In the simplest case, all particles are assumed to be identical, and no effects of chemistry or electrical charge are considered. Since the number of gas molecules is huge (10^{19} per cm^3 at standard conditions), it would be impossible to study the behavior of each individual molecule. Instead, a statistical description is used—some function $f(t,x,v)$ representing the relative amount of gas particles at time t having a position close to x and a velocity close to v.

The basis for this statistical theory was provided in the second half of the 19th century. James Clerk Maxwell found the distribution function of the gas molecule velocities in thermal equilibrium,

$$f_{eq}(v) = \frac{1}{[2\pi\, T]^{3/2}} \exp\left(-\frac{\|v\|^2}{2\,T}\right), \qquad v \in \mathbb{R}^3\,. \tag{1}$$

The number T corresponds to the temperature of the gas.

Fig. 2: *Ludwig Boltzmann (1844-1906)*

Ludwig Boltzmann studied the problem whether a gas starting from any initial state reaches the Maxwellian distribution (1). In [2] he established the equation

$$\frac{\partial}{\partial t} f(t,x,v) + (v, \nabla_x) f(t,x,v) = \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v,w,e)\Big[f(t,x,v^*)\, f(t,x,w^*) - f(t,x,v)\, f(t,x,w)\Big]\,de\,dw\,, \tag{2}$$

which governs the time evolution of the distribution function $f(t,x,v)$, where $t \geq 0$ and $x, v \in \mathbb{R}^3$. Here ∇ denotes the vector of partial derivatives, $(.,.)$ is the scalar product, and $\mathbb{S}^2$ is the unit sphere in the Euclidean space $\mathbb{R}^3$. The collision transformation

$$v^* = v^*(v,w,e) = v + e\,(e, w-v)\,, \qquad w^* = w^*(v,w,e) = w + e\,(e, v-w) \tag{3}$$

conserves momentum and energy. The collision kernel B is determined by the interaction potential between molecules. We refer to [3] concerning the history of kinetic theory.

The classical Boltzmann equation (2) is used in such applications where the mean free path (the average distance between subsequent collisions of molecules) is not negligible compared to the characteristic length scale of the problem. This means that either the mean free path is large, or the characteristic length is tiny.

A typical example with large mean free path is the reentry of a space shuttle into the atmosphere. Above an altitude of about 120 km the mean free path is larger than 1 m, and collisions between gas molecules can be neglected (free molecular flow). Below an altitude of about 70 km, the mean free path is smaller than 1 mm, and local equilibria are reached due to the huge number of collisions. The distribution function takes the form

$$f(t,x,v) = \frac{\rho(t,x)}{[2\pi\, T(t,x)]^{3/2}} \exp\left(-\frac{\|v - U(t,x)\|^2}{2\,T(t,x)}\right),$$

where $\rho(t,x)$, $U(t,x)$, and $T(t,x)$ are the local density, bulk velocity, and temperature, respectively. The time evolution of these macroscopic quantities is determined by the fluid dynamics equations. Instead of finding one function of seven variables, one has to find five functions of four variables each, which is much easier. Between the free molecular regime and the fluid dynamics regime, the Boltzmann equation is relevant. Its solution delivers the necessary input information for the fluid dynamics equations.

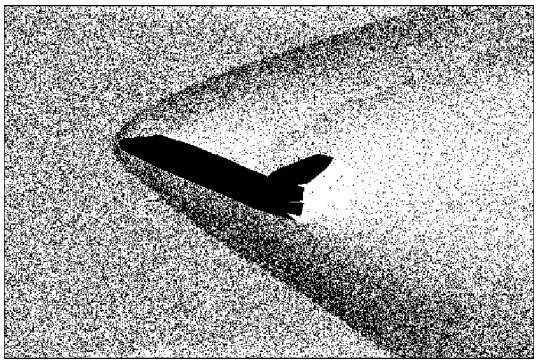


Fig. 3: *Shock profile of a shuttle reentry*

Another field of application where the mean free path is large, is vacuum technology (e.g., material processing via vapor deposition).

However, there are also applications in our common environment. At standard atmospheric pressure and temperature 20°C, the mean free path of an oxygen molecule is about 50 nm. The molecule travels at an average velocity of about 500 m/s suffering about 10^{10} collisions per second. Its diameter is about 0.3 nm, so that it travels a distance of 150 times its diameter between collisions. Applications with a tiny characteristic length scale are engineering of micro-electro-mechanical systems (MEMS) or calculating the flows in a disc drive (read/write head floats less than 50 nm above the surface of the spinning platter).

Stochastic interacting particle systems

Stochastic models for the Boltzmann equation are based on systems of particles

$$Z^{(n)}(t) = \Big(x_1(t), v_1(t); \ldots; x_n(t), v_n(t)\Big), \qquad t \geq 0\,, \tag{4}$$

imitating the behavior of the gas molecules in a probabilistic way. The main mathematical interest is in proving rigorously the convergence of the system (when the number of particles increases) to the solution of the equation in an appropriate sense. The study of the relationship between the process (4) and the Boltzmann equation (2) was started by M.A. Leontovich in the paper [4] in 1935.

Fig. 4: *M.A. Leontovich (1903–1981)*

Let $p^{(n)}(t,z)$ denote the n-particle distribution function of the process (4). Leontovich obtained the equation

$$\frac{\partial}{\partial t}\, p^{(n)}(t,z) + \sum_{i=1}^{n} (v_i, \nabla_{x_i})\, p^{(n)}(t,z) = \frac{1}{2n} \sum_{1\le i\ne j\le n} \int_{\mathbb{S}^2} \Big[p^{(n)}(t, J(z,i,j,e)) - p^{(n)}(t,z)\Big] q^{(n)}(x_i, v_i, x_j, v_j, e)\, de\,, \tag{5}$$

where the function $q^{(n)}$ governs the jump intensity and (cf. (3))

$$[J(z,i,j,e)]_k = \begin{cases} (x_k, v_k) & , \quad \text{if} \quad k \ne i,j\,, \\ (x_i, v^*(v_i, v_j, e)) & , \quad \text{if} \quad k = i\,, \\ (x_j, w^*(v_i, v_j, e)) & , \quad \text{if} \quad k = j\,, \end{cases}$$

is the jump transformation. Using the method of generating functions, he first studied the cases of "monomolecular processes" (independent particles) and of "bimolecular processes" with discrete states (e.g., a finite number of velocities). Under some assumptions on the initial state, he showed that the expectations of the relative numbers of particles in the bimolecular scheme asymptotically (as $n \to \infty$) solve the corresponding deterministic equation. In the case of the full Boltzmann equation, the stochastic process was described via (5) (even including a boundary condition of specular reflection). Concerning the asymptotic behavior of the process, Leontovich pointed out the following: Let $p_k^{(n)}$ denote the marginal distributions corresponding to the density $p^{(n)}$. If

$$\lim_{n\to\infty} p_2^{(n)}(t, x_1, v_1, x_2, v_2) = \lim_{n\to\infty} p_1^{(n)}(t, x_1, v_1) \lim_{n\to\infty} p_1^{(n)}(t, x_2, v_2)$$

and

$$\lim_{n\to\infty} q^{(n)}(x, v, y, w, e) = \delta(x-y)\, B(v, w, e)\,,$$

where δ denotes Dirac's delta-function, then the function

$$f(t,x,v) = \lim_{n\to\infty} p_1^{(n)}(t,x,v)$$

solves the Boltzmann equation. A review of the further development of the convergence theory is given in [5, Chapter 2].

Numerical algorithms and convergence

Since the dimensionality of the Boltzmann equation is high (time, space, velocity), its numerical treatment is a typical application field of Monte Carlo algorithms. The "direct simulation Monte Carlo" (or DSMC) algorithm is presently the most widely used numerical method in kinetic theory.

It goes back to papers on the homogeneous gas relaxation problem (1963) and the shock structure problem (1965) by G.A. Bird (cf. [1]). The development of the subject is also well reflected in the proceedings of the bi-annual international conferences on "Rarefied Gas Dynamics" ranging from 1958 to the present.

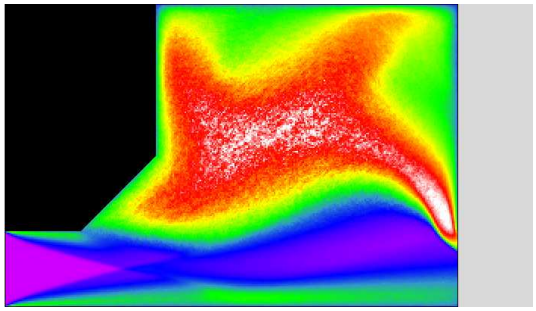


Fig. 5: *Temperature profile of a rocket plume*

The method is based on the process (4) but includes several numerically motivated modifications. Independent motion (free flow) of the particles and their pairwise interactions (collisions) are separated using a splitting procedure with a time increment Δt. During the free flow step, particles move according to their velocities,

$$x_i(t+\Delta t) = x_i(t) + \int_t^{t+\Delta t} v_i(s)\,ds\,, \qquad i = 1,\ldots,n\,,$$

and do not collide. At this step, boundary conditions are taken into account. During the collision step, particles do not change their positions. Here some partition of the spatial domain into a finite number of disjoint cells is introduced, which leads to a decoupling of collision processes in different cells. Convergence of the method was established in [6].

One of the most important theoretical issues in Monte Carlo theory is the problem of variance reduction. Applied to direct simulation schemes, it means that the "natural" level of statistical fluctuations should be reduced in order to better estimate certain average quantities. In rarefied gas dynamics, such quantities might be macroscopic characteristics of flows with high density gradients, or tails of the velocity distribution. Roughly speaking, variance reduction assumes having a parameter-dependent class of models approximating the same object. The parameter is then chosen in order to reduce the variance, thus improving the stochastic convergence behavior. In the linear case, all random variables usually have the same expectation, corresponding to the quantities of interest. In the nonlinear case, it is also necessary to make parameter-dependent models comparable. One way is to check that the random variables converge to the same limit, independently of the choice of the parameter.

The monograph [5] provides a comprehensive account of recent research activities in the area of stochastic numerical methods for the Boltzmann equation. The first goal of this book is to give a mathematical description of classical direct simulation Monte Carlo (DSMC) procedures for rarefied gases, using the theory of Markov processes as a unifying framework. The second goal is a systematic treatment of an extension of DSMC, called stochastic weighted particle method (SWPM). This method includes several new features, which are introduced for the purpose of variance reduction (rare event simulation). Rigorous convergence results as well as detailed numerical studies

are presented.

Following ideas used in the case of linear transport, a specific variance reduction strategy is to fill the position space (or larger parts of the velocity space) uniformly with particles, while the weights of these particles provide information about the actual density. In the general context, the uniformity corresponds to the introduction of some deterministic components (regular grid, order, etc.). SWPM is based on this strategy. The method consists of a class of algorithms containing certain degrees of freedom. For a special choice of these parameters the standard DSMC method is obtained. More general procedures of modeling particle collisions as well as inflow and boundary behavior are implemented. The degrees of freedom are used to control the behavior of the particle system, aiming at variance reduction. A systematic treatment of SWPM (including convergence theory) is given in [5, Chapter 3].

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2.2 Pulse Dynamics in Mode-locked Lasers for Optical Telecommunications

Andrei Vladimirov and Matthias Wolfrum

Introduction

Semiconductor laser devices, which are able to generate short optical pulses at high repetition rates, are key elements in modern optical communication systems. At present, our partners at Fraunhofer-Institut für Nachrichtentechnik Heinrich-Hertz-Institut (HHI), Berlin, are developing a mode-locked multi-section semiconductor laser that should be able to generate pulses of a length of less than 2 ps at a repetition rate of 40 GHz. Since experiments are quite expensive and time-consuming, HHI scientists are cooperating with WIAS, in order to obtain by mathematical modeling and simulation a better understanding of the complex internal processes in such devices and to get ideas for an optimized design for their components.

Multi-section semiconductor lasers are highly complex devices. Within their total size of 1 mm, they carry a complex structure, ranging from the geometry and multi-section structure of the whole device down to the nanostructures in the active material. There, so-called *quantum wells* with a size of a few nanometers are able to capture the electrons supplied by the driving current. Due to these localized electrons, a stimulated emission of light becomes possible that is able to sustain a lasing process. To this end, the emitted light has to be guided along the laser. This is achieved by a transversal structure with different refractive indices, similarly as in optical fibers. Finally, a multi-section laser is composed of different sections that can be controlled separately. Within these different sections, the propagating light can not only be amplified, but also manipulated in different ways, e.g., by optical gratings or saturable absorbers. By using specific multi-section structures, it is possible to design laser devices with specific dynamical properties for optical communication systems.

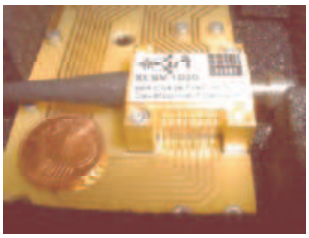

Fig. 1: *Mode-locked laser, developed at HHI*

For a mathematical treatment, the challenge is not the smallness of the devices itself, but the fact that the devices are structured on scales that differ by a factor of 10^6. At the same time, a variety of different physical effects are relevant for the operation of such a device that have to be taken into account for its mathematical description.

The challenge for an efficient mathematical modeling of such devices is to describe all the physical processes on the different scales in time and space and their interaction in a way that captures their relevant features and, at the same time, is simple enough to allow for a simulation on the computer and for a detailed mathematical analysis. In [1] we have introduced a novel system of so-called *delay differential equations* that is able to describe the mode-locking process in multi-section semiconductor lasers. Based on this mathematical model, it was possible to obtain a deeper theoretical understanding of the process of mode-locking and to find design rules for mode-locked lasers with a better performance in optoelectronic communication systems.

Pulse generation

The light in an optical waveguide with reflectivities at the ends of the cavity acts like a violin string or the air in an organ pipe: when energy is supplied, oscillations with definite wavelength occur. Like a tone with a fixed pitch of the violin or organ, a laser can produce constant coherent light having a fixed optical frequency. This is the well-known principle of a laser. But it does not explain why a laser can be made to generate short pulses.

The reason why a laser—in contrast to a violin or an organ—can produce something like short pulses can be explained as follows. It is well known that the oscillation of a string does not only contain a standing wave of the basic frequency, where the wavelength coincides with the length of the string, but also overtones, where multiples of the wavelength coincide with the length of the string. The mixture of these components creates the specific sound of each instrument.

The light in a laser has a wavelength in a range of nanometers, and hundreds of wavelengths fit into the cavity. In fact, in a laser there are many so-called *optical modes* having only slightly different frequencies and different numbers of wavelengths fitting into the cavity. And with these modes, it is possible to compose short pulses. To this end, it is necessary to adjust the phases of the modes in such a way that they interfere constructively at the pulse location and annihilate each other inbetween the pulses (see Figure 2). In this way, with an increasing number of locked modes, one can obtain shorter and higher optical pulses.

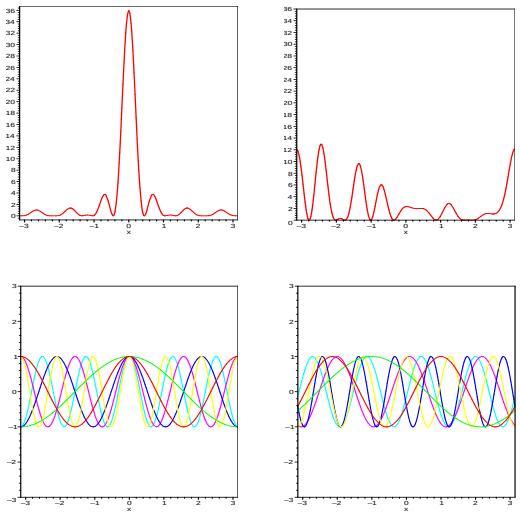

Fig. 2: *Composition of a pulse by superposition of modes with properly locked phases (left); irregular pattern for a superposition of the same modes with arbitrary phases (right)*

These pulses circulate in the cavity at the velocity of light and are emitted at the facet of the device through a mirror that reflects only a part of the light back into the cavity. Hence, the repetition frequency of the pulses is given by the velocity of light divided by the length of the laser. For a laser with a length of 1 mm, one obtains a frequency of 40 GHz that corresponds to 40,000,000,000 pulses per second.

The locking of the modes can be achieved by a process that is called *saturable absorption*. In one section of the laser the light is not amplified, but absorbed in a special nonlinear way. At high intensities, the absorption saturates, and pulses can pass, whereas constant emission is prevented

by the unsaturated absorption. But this mechanism also leads to other dynamical effects that can decrease the pulse quality or even become dominant over the mode-locking. It is the main goal of a mathematical investigation of the pulse dynamics to understand and to control these dynamical processes.

Pulse dynamics

The mathematical theory of nonlinear dynamical systems offers the opportunity to analyze the dynamical effects occurring in mathematical models describing the time evolution of physical systems. Transitions between regimes of different dynamical behavior are called *bifurcations*. Like the flow pattern from a water tap, which changes at a certain point from steady flow to dropping when the water pressure is decreased, the dynamical behavior of a system may change in a variety of possible ways. Besides the transition from stationary to periodic motion, mathematicians have investigated many other types of such bifurcations. By advanced mathematical methods, the conditions for a specific bifurcation can be extracted directly from the model equations, and the resulting bifurcation equations can be solved numerically on a computer.

In this way, one obtains so-called *bifurcation diagrams* showing how the dynamical behavior depends on several control parameters in the system. In a mode-locked laser the main parameters that can be tuned in the experiment are the electrical currents for optical gain and saturable absorption. In addition, there is a large number of parameters related to the design of the laser that can be changed only by producing new devices.

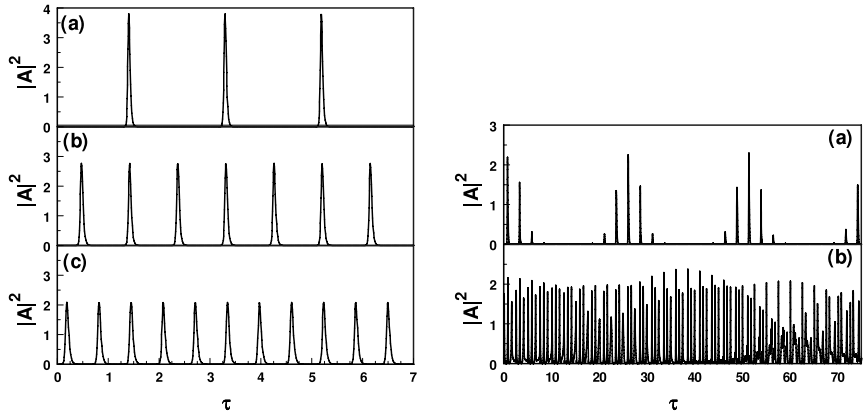

Fig. 3: *Dynamical regimes of mode-locked lasers. Left: subharmonic mode-locking. Right: periodically (a) and chaotically (b) modulated mode-locking.*

Besides the operation of mode-locking, the following dynamical regimes can be found.

- Stationary lasing
- Emission of single pulses at a low repetition rate, so-called *Q-switching*
- Subharmonic mode-locking, where more than one pulse circulates in the cavity and multiples of the mode-locking repetition frequency can be observed (see Figure 3, left)
- Complicated dynamics, where the mode-locking pulsation can be modulated chaotically or periodically by the Q-switching process (see Figure 3, right)

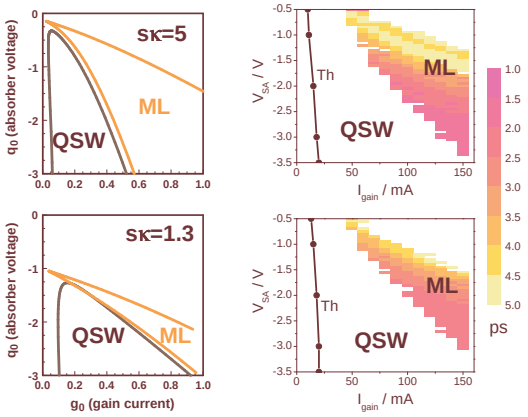

Fig. 4: *Larger regions with stable mode-locking (ML) for lasers with optimized design (upper figures). Theoretical prediction (left), experiment (right)*

By calculating the corresponding bifurcations, we were able to identify the processes that lead to limitations in the quality of the mode-locking pulses and to understand their dependence on the design of the device. In this way we obtained design rules for an optimized device, which have been used by our cooperation partners at HHI.

The left part of Figure 4 shows calculated bifurcation diagrams for different designs of the mode-locked laser. The curves determine the parameter regions where a certain dynamical behavior can be found. The laser with the optimized design (upper diagram) shows a considerably larger region of stable mode-locking (ML), whereas the region with the undesirable Q-switching (QSW) has been decreased compared to the initial design (lower diagram). The experimental data in the right part of Figure 4 show the improved performance of the devices with the new design, fabricated at the Heinrich-Hertz-Institut. These devices now satisfy the quality requirements needed in systems applications.

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2.3 Regularity for Elliptic and Parabolic Differential Equations

Johannes Elschner, Hans-Christoph Kaiser, Joachim Rehberg, and Gunther Schmidt

The history of partial differential equations goes back more than 250 years: the one-dimensional wave equation modeling a vibrating string,

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2},$$

was originated by d'Alembert in 1752 and analyzed in the following years. His work has been extended by Euler (1759) and by D. Bernoulli (1762) to the two- and three-dimensional wave equations in the study of acoustic waves. A few years later, Laplace, in his work on gravitational fields, established and first studied the equation

$$\Delta u = 0,$$

which since then carries his name. The heat equation,

$$\frac{\partial u}{\partial t} = \Delta u,$$

was introduced by Fourier in his "Théorie Analytique de Chaleur" (1810–1822). Thus, problems in physics, and later on in chemistry, biology, and technology, have been the original sources for partial differential equations (PDEs), and to a large extent remained this for the progress in this field. On the other hand, until today partial differential equations form, besides modern stochastics, the most adequate and powerful instrument to provide a mathematical model for nature. Besides, it turned out that there were many connections to other branches in mathematics, such as differential/algebraic geometry, algebraic topology, etc. For further historical remarks, see [1].

The above examples of PDEs are of *hyperbolic*, *elliptic*, and *parabolic* type, respectively. It was understood relatively early, and systematically investigated beginning with Hadamard (1923), that linear partial differential equations can (mainly) be classified as elliptic (Laplace's equation), parabolic (heat equation), and hyperbolic (wave equation), and that to each of these classes associated boundary or/and initial conditions have to be imposed. For example, among the second-order equations the elliptic ones have to be complemented by suitably prescribed boundary data, the parabolic ones by suitable boundary data and a condition for the initial time, while hyperbolic equations have to be supplemented by data for the initial position and the initial velocity, prescribed on a noncharacteristic manifold. This being understood, the following questions are of interest:

I. Does the corresponding partial differential equation possess a solution?
II. If the solution exists, is it unique?
III. Do the solutions depend continuously on the data of the problem?
IV. How regular (analytic, differentiable, continuous ...) is the solution?
V. Are there adequate numerical procedures to approximate the solution?

Meanwhile, it is well understood that these questions are highly interrelated; in particular, the knowledge of regularity often is of help concerning II, III, and V.

The first wide-ranged regularity result was proved in 1875 by Kovalevskaya. It states, roughly speaking, that if the coefficients and the initial data of a partial differential equation are analytic, then the solution exists locally and is itself analytic.

In 1900, Hilbert in a famous talk posed two problems that explicitly affected the question of regularity of solutions. Especially, "Problem 19" is of interest to us: is the solution of a fully nonlinear elliptic problem in the plane,

$$F(x, y, u, Du, D^2u) = 0\,,$$

analytic whenever F is? It was Bernstein who proved in 1904 that any C^3 solution is in fact analytic. Besides, Hilbert's formulation of regularity nowadays serves as a prototype: the principal question is how regular the solutions of a partial differential equation are in their dependence on underlying domain, coefficients, and initial/boundary data. What needs clarification in this connection is the word "regular" itself. Let us start with two examples:

1. Consider the function $u : (x, y) \mapsto \Im(\sqrt{x+iy})$. It is harmonic in the upper half plane and satisfies the following homogeneous boundary conditions on the real line:

$$u = 0 \quad \text{for } x > 0\,, \quad \text{and} \quad \frac{\partial u}{\partial y} = 0 \quad \text{for } x < 0.$$

Despite the fact that the data of the problem, namely domain, Dirichlet, and Neumann data, are arbitrarily smooth (namely zero), it can easily be seen that the partial derivatives of first order are not summable with exponent 4 (see also Figure 1).

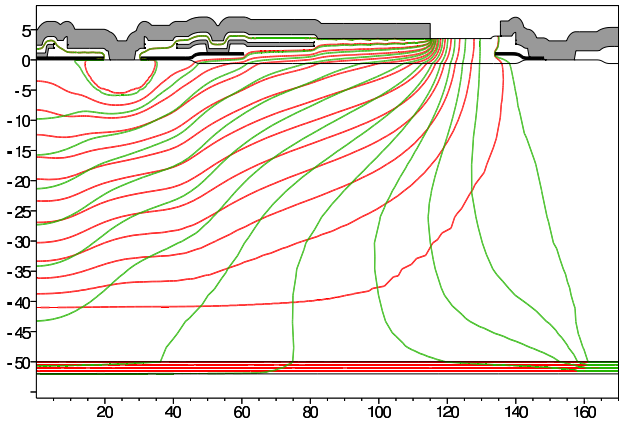

Fig. 1: *WIAS-TeSCA simulation of the cross section of a transistor: isolines of the electric field. The compression at the transition between contact (Dirichlet boundary) and insulator (Neumann boundary) indicates steep gradients of the electrostatic potential.*

2. Consider as domain Ω the wedge $\{(x, y) : 0 < \arg(x+iy) < \alpha\}$. Then the function

$$(x, y) \mapsto (x^2 + y^2)^{\lambda/2} \sin(\lambda \arg(x+iy))\,,$$

with λ taken as $\frac{\pi}{\alpha}$, is harmonic on Ω and vanishes on the boundary rays $y = 0$ and $y = x \tan \alpha$. As is easy to check, its partial derivatives are (locally) summable only up to an exponent $\frac{2}{1-\lambda}$.

Both examples show that, in spite of regular data, the partial derivatives of the solutions are not

bounded and cannot be extended up to the boundary, even though they are solutions of an elliptic second-order equation. In the first case, this is due to the mixed boundary conditions, while in the second the corner of the domain at zero is responsible for this effect. This means that the mathematical notions of continuous differentiability (also Hölder continuity) are not sufficient to describe the regularity of solutions for frequently occurring problems.

It have been the notions of *distributions*, of *weak solutions*, and of *Sobolev spaces*, which brought order into this confusion. For example, a function u is called a weak solution of the equation $-\mathrm{div}(\mu \,\mathrm{grad}\, u) = f$, if for any C^∞ function ψ with compact support the integral relation

$$\int_\Omega \mu \nabla u \cdot \nabla \psi \,\mathrm{d}x = \int_\Omega f \psi \,\mathrm{d}x \tag{1}$$

is true. This formulation is based on the observation that any classical solution is, by partial integration, also a weak one. Reversely, this weak formulation for the first time really enabled a precise formulation of, say, an elliptic equation with discontinuous coefficient function μ. This turned out to be absolutely essential in many modern applications. Moreover, the right-hand side of (1) might also not be a usual function, but, for example, a surface density (in which case the integral on the right-hand side of (1) has to be replaced by a surface integral). Having this framework at hand, the study of PDEs could be performed in two steps: First prove the existence of a weak solution, then show that the weak solution admits more regularity, at best is a classical solution.

In case of elliptic and parabolic equations, this program works. In particular, if the underlying domain is smooth, if the coefficients are Hölder continuous, and if the initial/boundary data are smooth, then weak solutions are classical ones, owing to the Weyl lemma. If the coefficients are bounded and elliptic, then according to de Giorgi, Nash, and Moser, it can be proved that the weak solution is Hölder continuous. Another mathematical instrument that highly served as an ordering principle and turned out to be adequate for the treatment of many problems was the notion of Sobolev spaces (1938). What make them such powerful instruments are (among other things) the famous Sobolev embeddings.

At WIAS, elliptic and parabolic equations are of particular research interest, since they occur in many application areas: phase field models, phase separation, modeling of semiconductors (see Figures 1 and 2), of crystal growth, and of the hysteretic behavior of shape memory materials. For the treatment of such equations, the Sobolev spaces $W^{1,q}(\Omega)$ often are the adequate regularity class. They are defined as the completion of the class of C^∞ functions with respect to the norm

$$u \mapsto \Big(\int_\Omega (|\nabla u|^2 + |u|^2)^{q/2} dx\Big)^{1/q},$$

their subspaces

$$W^{1,q}_\Gamma(\Omega) := W^{1,q}(\Omega) \cap \{\psi \,:\, \mathrm{tr}\ \psi = 0 \text{ on } \partial\Omega \setminus \Gamma\}\,,$$

and the duals $W^{-1,q}_\Gamma(\Omega) := \Big(W^{1,q'}_\Gamma(\Omega)\Big)^*$. Notice that

$$\langle -\mathrm{div}(\mu \,\mathrm{grad}\, u), \psi\rangle = \int_\Omega \mu \nabla u \cdot \nabla \psi \,\mathrm{d}x \qquad \text{for all } \psi \in W^{1,q'}_\Gamma(\Omega)\,,$$

gives a precise definition of the operator

$$A := -\mathrm{div}(\mu\,\mathrm{grad}) + 1 : W_\Gamma^{1,q}(\Omega) \to W_\Gamma^{-1,q}(\Omega). \tag{2}$$

It is well known from the famous Lax–Milgram lemma that $-\mathrm{div}(\mu\,\mathrm{grad}) + 1$ always provides a topological isomorphism if $q = 2$. More generally, in case of smooth domains Ω and, say, Dirichlet boundary conditions, it has also been known for a long time that the Laplacian provides a topological isomorphism between $W_0^{1,q}(\Omega)$ and $W^{-1,q}(\Omega)$ or, alternatively, between $W^{2,q}(\Omega) \cap W_0^{1,q}(\Omega)$ and $L^q(\Omega)$ for all $q \in]1, \infty[$. The serious shortcoming is the fact that these results are limited to the case of smooth domains, constant (or at least continuous) coefficients, and only one sort of boundary conditions: either Dirichlet or Neumann; see the examples above. In particular, one never recovers quadratic summability for the second derivatives in the case of discontinuous coefficients. On the other hand, in applications in technology and in the modeling of heterogeneous structures (such as in mechanics, thermodynamics, electrodynamics, quantum mechanics), one is very often confronted with nonsmooth domains, jumping coefficients, and/or mixed boundary conditions (see Figure 2). In particular, in semiconductor device simulation by means of van Roosbroeck's system, operators of type (2) are of relevance. Here, heterostructures are the determining features of many fundamental effects. With the ongoing miniaturization of electronic devices, the resolution of material interfaces becomes ever more important, so that one definitely has to deal with discontinuous coefficients.

During the past two decades, it turned out that for many applications, especially in case of nonlinear problems, the knowledge that (2) also provides a topological isomorphism for a q larger than the dimension of the underlying domain Ω is of great use: on the one hand, the uniqueness for associated nonlinear problems is implied, on the other hand, this turned out to be of great interest for the treatment of semilinear and even quasilinear parabolic equations. In 1989, Gröger proved this for a $q > 2$ for Lipschitz domains Ω under very general conditions on the Neumann boundary part. This result solved the two-dimensional case and was applied to many problems. Working on the Sobolev–Campanato scale, Griepentrog could extend de Giorgi's theorem, which asserts the Hölder continuity for solutions of the Dirichlet problem (adequate right-hand sides supposed), to the case of mixed elliptic boundary value problems with discontinuous coefficients.

Concerning the isomorphism property (2), it has been known for long that it is only true for $q = 2+\epsilon$ with arbitrarily small $\epsilon > 0$ in general. Therefore, the fundamental question for three-dimensional problems reads:

Is it true, for sufficiently many practically relevant elliptic operators (including nonsmooth domains Ω, mixed boundary conditions, and discontinuous coefficient functions μ), that (2) provides an isomorphism for a $q > 3$?

The answer is "yes" if the domain has a Lipschitz boundary, the coefficient function is continuous, and the Dirichlet and Neumann parts of the boundary "meet suitably." What has not been treated thus far in the non-Hilbert space scale, is the case where interfaces of discontinuities for the coefficient function μ are nonsmooth or/and meet with the boundary. Let us give the results that were derived for this case over the past three years (see [3]):

Theorem: Let Ω be a polyhedron, and let a decomposition of Ω into subpolyhedra be given. Assume that the coefficient function μ is constant on every subpolyhedron, and attains its values in the set of real, positive definite matrices. Associate to every (inner and outer) edge generated by the decomposition a suitable two-dimensional problem. If the singular exponents of all these associated two-dimensional problems are larger than $1/3$, then (2) is an isomorphism for some $q > 3$.

Thus, this theorem allows to avoid the complicated discussion concerning corner singularities, provided that the edge singularities can be controlled in the spirit of the theorem. It remains to supply sufficient conditions on the geometry of Ω, on the partition, and on the assigned matrices on the subdomains that assure the suppositions of the above theorem. We could prove that these are always fulfilled in case of layered structures, and also in the case that the matrices occurring in the auxiliary two-dimensional problems satisfy certain order relations. The latter gives hope for a successful treatment of structures as in Figure 2.

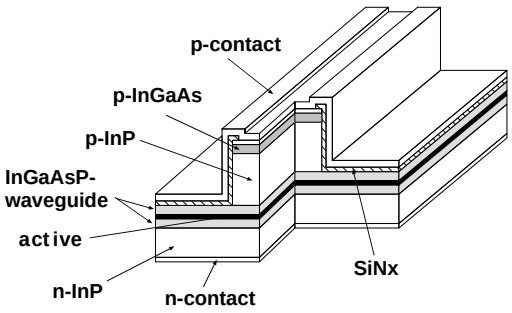

Fig. 2: *Multi-quantum-well laser*

For parabolic problems, often the setting

$$\frac{\partial}{\partial t} - A : W^{1,r}(S, X) \cap L^r(S; \mathrm{dom}(A)) \cap \{w : w(0) = 0\} \to L^r(S; X), \tag{3}$$

where X is an appropriate Banach space and A is an elliptic operator with domain $\mathrm{dom}(A)$, is adequate for the treatment of nonlinear problems. In particular, this is true in the case that the right-hand side depends explicitly and discontinuously on time, which is often relevant in technology. The reader should, e.g., think of a manufacturing process for semiconductors, in which at a certain moment light is switched on/off, and, of course, parameters in the description of the chemical process change abruptly. The crucial point is to prove that (3) is a surjection and, hence, that the operator $\frac{\partial}{\partial t} - A$ is an isomorphism or, in other words, satisfies maximal regularity. It has been proved last year that in the case $X = L^p$ and of operators A of the type $\alpha\ \mathrm{div}(\mu\ \mathrm{grad})$ (including mixed boundary conditions, discontinuous coefficients), α being a positive and bounded function, $\frac{\partial}{\partial t} - A$ in fact satisfies maximal regularity. Having this at hand, even doubly nonlinear parabolic equations/systems can be treated. For some of our results in this direction, we refer to [2], [3].

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2.4 Phase Transitions and the Evolution of Precipitates in Crystalline Solids

Wolfgang Dreyer

Phases and phase transitions

All matter in our surroundings may occur in the three possible states *solid, liquid, and gas*. These states of the matter are called the *phases*. Depending on some control parameters, a given substance may change its phase, and we refer to this process as a phase transition. The freezing of water may serve as a prominent example. If the temperature at the surface of a liquid lake falls below 0°C, a thin sheet of ice is formed that subsequently grows towards the bottom of the lake. Thus for a certain time, a body with two coexisting phases has formed, and these are separated by a more or less flat interface.

Precipitates

Presumably the most familiar precipitates in a given substance are small liquid droplets formed in wet air, commonly called *fog*. The objective to model and simulate the evolution of fog under given boundary conditions is one of the tasks of thermodynamics. A more complex situation is seen with crystalline solids, where under certain conditions the appearance of liquid precipitates might likewise be possible.

Some characterizations of the phases

The phases solid, liquid, and gas, exhibit enormous differences in their atomic constitution, and they behave differently in physical processes. The gas atoms undergo mostly a free-flight motion, and the interaction of two atoms is quite a rare event. For example, the mean time of free flight in air at 20°C and at 1 bar is about 10^{-9} s, and the duration of an interaction is even shorter by a factor of 3,000. The liquid atoms have much shorter distances from each other, and thus there is a continuous interaction between them. The different mean distances between gas and liquid atoms can be calculated from their specific volumes, which give the volume that a single atom has at its disposal. Under conditions in which gaseous and liquid phases of water coexist at 100°C, the specific volume of the gas phase is 1,000 times larger than that of the liquid phase. At 2°C this difference is even 170,000. The mean distances of solid and liquid atoms are comparable. The most apparent difference between the solid and the liquid and gas phase, respectively, is its response to mechanical loading. Liquids and gases do not resist changes of the geometric shape of their volume. Exclusively changes of the size require external work. In contrast, the deformation of the shape of solids also gives rise to stresses.

Mathematical modeling of phase transitions

At WIAS, we model the evolution of phase transitions and, in particular, of precipitates on various time and length scales. The equations of motion for individual particles on the atomic scale consist of large systems of nonlinear ordinary differential equations, and they form the fundamental basis for modeling. However, we do not try to solve these equations; they rather serve to motivate the structure of a few partial differential equations that govern the evolution of phase transitions on the macroscopic scale, which may range from µm to mm. Here, we describe the atomic motion in the mean by nonlinear diffusion equations driving the evolution. These equations are coupled to quasi-static momentum equations that take care of mechanical stress fields that are very likely to appear during phase transitions.

There are two methods to describe the morphology, i.e., the spatial distribution of different phases. The boundary between two adjacent phases may be treated explicitly by boundary conditions. In this case, the interface forms a hypersurface on which some of the variables suffer a discontinuity. The mathematical problem at hand is called a *free boundary problem*, because the evolution of the boundary between two phases is a priori unknown and thus part of the solution of the full problem. The second method prefers to avoid variables with discontinuities. Here, the spatial transition layer between two phases has a thin but finite extent. In this region, the variables change smoothly according to partial differential equations that contain the information of the boundary conditions of the first method.

In the following, we give three typical examples to illustrate special phenomena in connection with phase transitions, in which the characteristic strategy of the Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*, to unify multiscale modeling, analysis, and simulation of phase transitions, is applied. The first example concerns phase transitions in steel. Here, the mathematical model consists of a free boundary problem for a diffusion equation with thermomechanical coupling. Next, the behavior of solder materials in microelectronic devices is described, where the mathematical model leads to a phase field model that is used to simulate the interior of the solder, and a free boundary model suited to describe the interface between the solder and, say, a copper pad. Finally, we introduce quite a complex phenomenon that occurs during the production process of gallium arsenide wafers. It concerns the appearance of undesired liquid precipitates in a given crystalline surrounding. The modeling requires the consideration of various time and length scales. For example, the vicinity of a single precipitate is modeled by a nonlinear diffusion equation containing inhomogeneous stress fields. The evolution of the size distribution of a system with many precipitates is described by a large system of ordinary differential equations of so-called Becker/Döring type, and the simulation of the spatial distribution of the precipitates requires homogenization techniques. These complexities necessitate the collaboration with external research groups within the DFG Research Center MATHEON.

Phase transitions in solids. Part 1: Steel

A thermodynamics study of a solid reveals that many different solid phases may occur in nature. For example, steel consists of iron and carbon atoms. The iron atoms are periodically arranged

in crystal lattices with a certain symmetry, whereas the carbon atoms might be considered as a gas that lives on interstitial sites of the iron lattice. The crystal symmetry is determined by the temperature and by the fraction of carbon atoms that are locally present. The following simplified picture serves as an illustration.

At high temperature, and for high carbon content, the iron forms a lattice with a *face-centered cubic* (fcc) symmetry, i.e., the unit lattice cell is a cuboid having eight iron atoms at the cell corners and six iron atoms at the centers of the six cell faces. If the fraction of carbon atoms is now drastically decreased at fixed temperature, then the iron atoms rearrange to form a new lattice with a *body-centered cubic* (bcc) symmetry. Here, the unit cell is still a cuboid, but with an iron atom at the center of the cell and no atoms at the faces. These two states constitute two solid phases of steel, which are called *austenite phase* and *ferrite phase*.

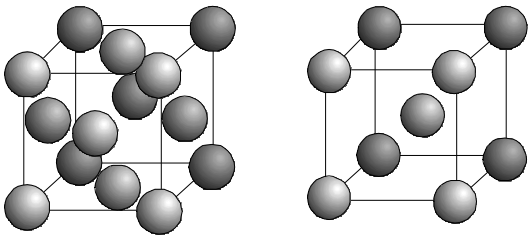

Fig. 1: *Possible unit lattice cells of steel; left: austenite, right: ferrite.*

There is a region in which the content of carbon is between these two extremes, and here both phases may coexist. If this region is reached by lowering the temperature at fixed mean carbon concentration, then the austenite phase appears as precipitates in the surrounding ferrite phase. Note that many more than just these two phases may occur in steel.

Phase transitions in solids. Part 2: Tin-lead solders

A further example for possible solid phases is provided by a solder material that is used to establish the electrical and mechanical connections of different microelectronic devices. In the recent past, the commonly used solder has been a tin/lead alloy with a 61.9% mean fraction of tin.

The production of the solder starts at a high temperature at which the constituents tin and lead are homogeneously distributed in the liquid phase. Lowering the temperature below the melting temperature, which is 168°C, leads to a solid phase with an inhomogeneous distribution of the two constituents. There are regions with high lead and high tin concentrations, and these regions form the α-phase and the β-phase. The structure occurring on the µm scale of the virgin state is controlled by the cooling rate. A possible microstructure might be a fine mix of alternating α-phase and β-phase layers. The crystal lattice of pure lead and pure tin has a face-centered cubic and tetragonal symmetry, respectively, and these properties are preserved in the α-phase and in the β-phase. The phase fraction, i.e., the amount of the β-phase, is determined by the temperature.

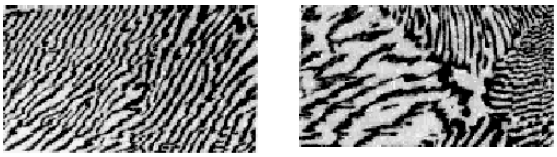

Fig. 2: *Morphology of α- and β-phases in a tin-lead solder. Left: virginal microstructure at 20°C; right: after some time at 100°C.*

In practical operation, the solder is exposed to external thermomechanical loading. For example, the micromechanical device may heat up from 20°C to 125°C, and this gives rise to mechanical stresses in the two phases of the solder, because the resulting thermal expansion is different in the two phases. This leads to undesirable changes of the morphology of the phases, so that a failure of the device becomes very likely.

Phase transitions in solids. Part 3: Semi-insulating gallium arsenide

Single crystal semi-insulating gallium arsenide (GaAs) is used as a substrate material for opto-electronic devices. This application requires a crystal of high purity and an extremely homogeneous distribution of its electrical properties.

The ideal GaAs crystal contains equal amounts of gallium and arsenic, living on a crystal lattice of so-called *zinc-blend symmetry* that can be described by a combination of three face-centered cubic sublattices of the same size. The sublattices are indicated by the letters α, β, and γ. In the ideal crystal the gallium atoms exclusively live on the α-lattice, whereas the arsenic atoms are exclusively found on the β-lattice, and the γ-lattice is empty. However, it is necessary to express this latter statement in different words: the γ-lattice is exclusively occupied by vacancies. Thus, solid GaAs is considered as one body with three constituents: gallium, arsenic, and vacancies. The vacancies are massless particles, but they are carriers of energy and of further thermodynamic properties.

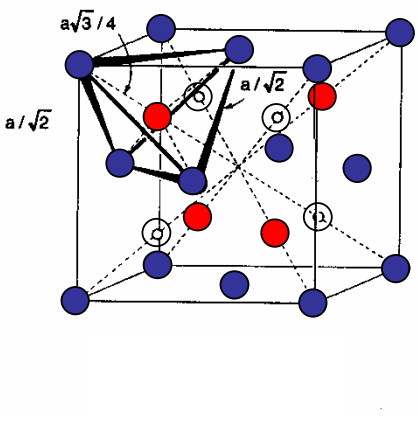

Fig. 3: *Sublattices of GaAs. Red: α-, blue: β-, white: γ-sublattice.*

For the production of semi-insulating GaAs, the symmetry of equal fractions of gallium and arsenic atoms must be slightly broken. For example, the arsenic fraction is increased from 0.5 to 0.500082 so that the gallium fraction is now 0.499918, which leads to a different distribution of the three

constituents on the three sublattices. Due to the size of the gallium atoms, these still can only reside on sublattice α. However, the arsenic and the vacancies may occupy all three sublattices. A careful study of the resulting phenomena reveals that the three constituents behave differently on the three sublattices, and an appropriate thermodynamic modeling of semi-insulating GaAs must take into account that there are thus seven different constituents. These are indicated by Ga_α, As_α, V_α, As_β, V_β, As_γ, V_γ. The constituents can move within the sublattices according to the laws of diffusion, and they can transfer between the sublattices, whereby their properties change in a chemical reaction.

A necessary heat treatment of the crystal is among the various steps to produce homogeneous semi-insulating GaAs. This happens at such a high temperature that the solid phase can coexist with the liquid phase, which appears in form of small liquid precipitates. Obviously, these precipitates are undesirable. Thus, a subsequent process must be designed that leads either to their dissolution or at least to a homogeneous distribution if dissolution is impossible.

Energy and entropy

The course of a phase transition and its equilibrium states are determined by an interplay of *energy* and *entropy*. Alongside with temperature, these are the key quantities of thermodynamics.

The energy consists of the kinetic energy of the irregular motion of the atoms, which is determined by the temperature, and further contributions, which measure the atomic interactions. Among these are *mechanical energies* originating from the distortion of the crystal lattice or from a change of the volume, *chemical energies* due to the release of heat in a chemical reaction, *diffusional energies* caused by the diffusional motion of the different constituents of the considered body, and *interfacial energies* due to the unbalanced interaction of the atoms in the interface of two adjacent phases.

The entropy, which is the other key quantity of thermodynamics, has a simpler meaning. It measures the degree of disorder. For example, a homogeneous crystal lattice at zero temperature and with all atoms at their ideal lattice sites, has zero entropy. In order to calculate the entropy for semi-insulating GaAs, one has to count in how many ways a given set of the seven constituents can be distributed over the three sublattices. The logarithm of that number gives the entropy.

Energy and entropy determine the evolution of a phase transition, and, in particular, the appearance and disappearance of precipitates, according to the following thermodynamic principles. The energy directs the process to states that minimize energy, while the entropy prefers states having maximal entropy. These two tendencies may come into conflict, and, in general, there is a competition on the significance of the principles of energy and entropy. At sufficiently low temperature, the energy principle wins, whereas the entropy principle directs the thermodynamic process at high temperature. In case that a phase transition occurs at constant temperature T and constant total volume V, the energy E and the entropy S form the so-called *free energy* $\psi = E - TS$, and all occurring processes run in such a way that ψ decreases monotonically and attains its minimum in equilibrium.

Mathematical capability to model, simulate, and optimize phase transitions

The two last examples reveal that there are undesired phase transitions in technologically important materials.

The microstructure of solder materials changes in an unfavorable manner due to the high service temperature. This problem cannot be solved by choosing other solder materials with a higher melting temperature, which would increase the durability in service, because the production process of the microelectronic connections needs low melting temperatures. This conflict can be studied and resolved by atomically-based thermodynamic modeling. The subsequent analysis of the mathematical equations allows to simulate all aspects of phase transitions and to identify the key parameters that are responsible for desirable and undesirable processes.

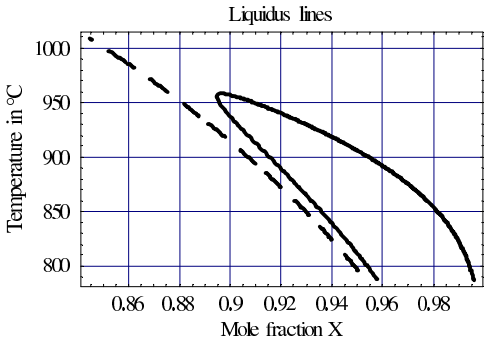

Fig. 4: *Lines of existence of liquid GaAs. Dashed and solid lines, respectively: liquidus lines without (dashed) and with (solid) mechanical and interfacial energies.*

The appearance of undesired liquid precipitates in semi-insulating GaAs may serve as a further example to illustrate the need for bringing physicists, engineers, and mathematicians together in order to treat and solve complex phenomena in modern materials.

At first, the precipitates appear during the heat treatment due to fluctuations of the local concentration of the arsenic. This is accompanied by an increase of energy, because interfacial energy has been created, and from this exclusive viewpoint, the energy principle prefers the dissolution of the precipitate. A further mechanism can be identified that also prefers dissolution: the liquid phase needs a little bit more space than the solid phase, so that the precipitate generates a mechanical stress field in the surrounding solid phase, which likewise leads to an unfavorable increase of energy. Furthermore, a growing precipitate annihilates vacancies, whereby the degree of disorder, i.e., the entropy, will be decreased. However, a liquid phase has higher entropy than a solid phase, and thus from the exclusive viewpoint of the entropy principle further growth of the precipitate is preferred.

Hence, the existence of a variety of competing mechanisms for and against the growth of a precipitate implies that only a systematic mathematical study allows to identify the key control parameters in the model equations to control the process appropriately. However, not every control parameter is easily adjustable in the production process, which shows again that only interdisciplinary studies with collaborations between physicists, engineers, and mathematicians will lead to significant improvements. In the current case, a study of various involved relaxation times, which

describe the speed of the approach to equilibrium of the processes discussed above, has led to an appropriately chosen temperature history.

2.5 Analysis and Numerics for Nonlocal Phase Separation Processes

Klaus Gärtner and Jens A. Griepentrog

Many interesting processes in physics take place in a closed system, with interacting particles of different type occupying a spatial domain. We are interested in describing processes like phase separation in alloys and demixing of gases and fluids on a many-molecular scale. Here, the averaged interaction forces are explicitly described by attractive interaction potentials for particles of the same type. The short-range repelling forces are accounted for using the distribution function of the so-called *Fermi–Dirac statistics*. This mesoscopic scale is larger than the single particle picture, and smaller than the continuum mechanics limit. Regarding a noisy image as a multicomponent mixture of colored particles is very natural from that point of view. The long-range forces are responsible for the agglomeration of particles of the same type—an enhancement of contrast from the viewpoint of image processing. On the other hand, the diffusion process ensures noise reduction as the following pictures show:

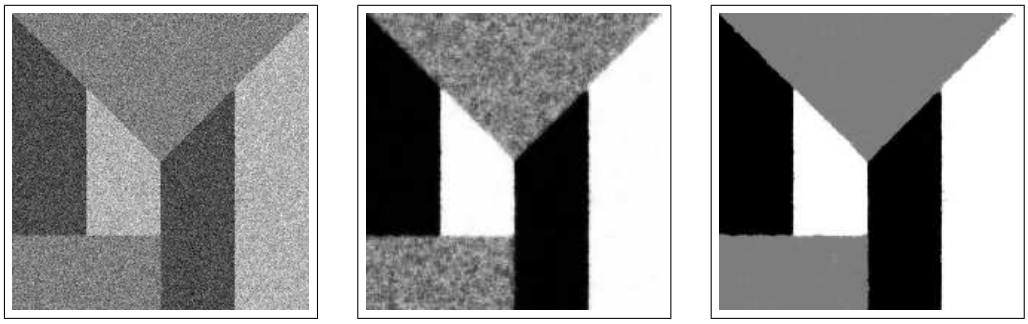

Fig. 1: *Image reconstruction for a strongly denoised 200 by 200 pixel image: (a) Initial value, noisy image; (b) final state of two-component black and white reconstruction, gray region still noisy; (c) final state of three-component black, white, and medium gray reconstruction.*

In a joint BMBF project with collaborators from the *Institut für Medizinische Physik und Lasermedizin* of the *Charité Universitätsmedizin Berlin*, we use the above nonlocal image segmentation method to analyze medical images regarding the scattering light distribution of the near-infrared spectral range on rheumatoid finger joints. Rheumatoid arthritis is the most common inflammatory arthropathy; it often affects the small joints, especially the finger joints. Inflammation of joints caused by rheumatic diseases starts with an inflammatory process of capsule synovial structures. Later, granulation tissue develops in the synovialis that destroys the cartilage and even the bone structure. Figure 2 shows two examples of healthy and rheumatoid finger joints, and the corresponding results of image segmentation with respect to three components (bone, cartilage, and synovial fluid). The final goal in this medical application is to accelerate the process of choosing suitable drugs from the many alternatives for the specific patient.

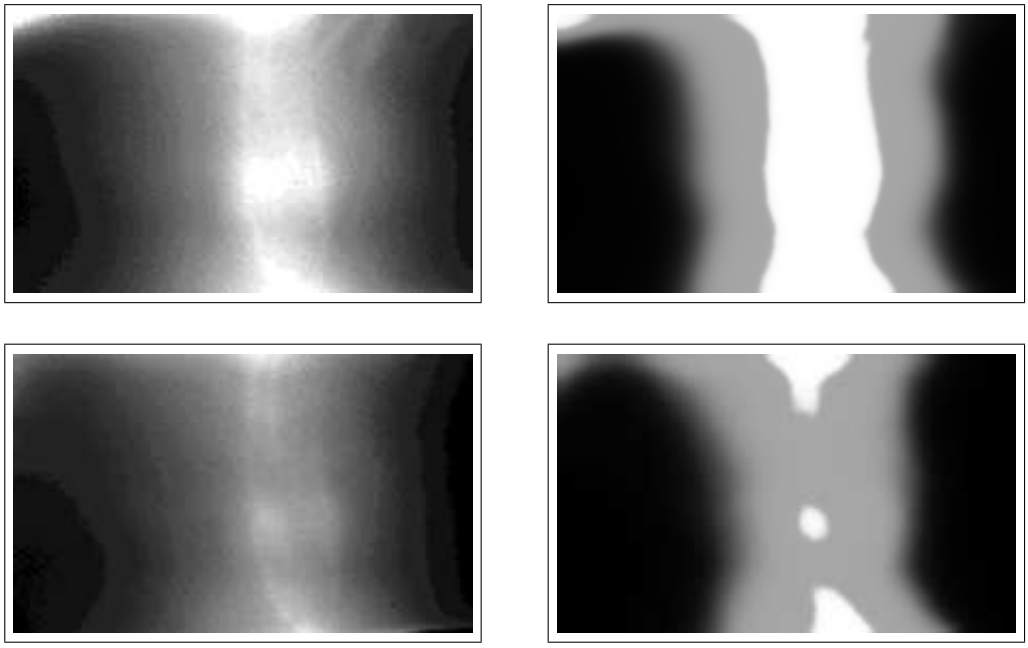

Fig. 2: *Image segmentation for scattering light images of human finger joints with respect to the three components bone (black), cartilage (gray), and synovial fluid (white): (a) Image of a healthy finger joint; (b) result of segmentation; (c) image of a rheumatically diseased finger joint; (d) result of segmentation.*

In the following, we give a brief summary of the model, and we illustrate the connection between its analytical and numerical stability properties. Finally, we show some numerical examples.

In our model, we assume that the particles jump around on a given microscopically scaled lattice following a stochastic exchange process. Exactly one particle sits on each lattice site (exclusion principle). Two particles of type i and $\ell \in \{0, 1, \dots, m\}$ change their sites x and y with a certain probability $p_{i\ell}(x, y)$, due to *diffusion* and *interaction*. The symmetric, reversible, and translation-invariant process tries to minimize the *free energy* of the particle ensemble occupying a spatial domain $\Omega \subset \mathbb{R}^n$. Then, the hydrodynamical limit; see [3], leads to a system of $m + 1$ conservation laws:

$$\begin{cases} u_i' + \nabla \cdot j_i = 0 & \text{in } (0, T) \times \Omega, \\ \nu \cdot j_i = 0 & \text{on } (0, T) \times \partial\Omega, \\ u_i(0) = u_i^0 & \text{in } \Omega, \end{cases} \tag{1}$$

with (scaled) *mass densities* $u_0, \dots, u_m$, their *initial values* $u_0^0, \dots, u_m^0$, and *current densities* $j_0, \dots, j_m$. Due to the exclusion principle, we have

$$0 \le u_i \le 1, \quad \sum_{i=0}^{m} u_i = 1, \quad \sum_{i=0}^{m} j_i = 0. \tag{2}$$

Here, only m of the $m + 1$ equations are independent of each other. We thus describe the state of the system by $u = (u_1, \dots, u_m)$ and $u_0 = 1 - \sum_{i=1}^{m} u_i$.

Physically relevant equilibrium distributions $u^* = (u_1^*, \dots, u_m^*)$ of the multicomponent system, and more generally, steady states of the evolution system, are supposed to be *local minimizers* of the

free energy functional F under the constraint of mass conservation,

$$\int_\Omega u(x)\,dx = \int_\Omega u^0(x)\,dx, \tag{3}$$

or solutions (u^*, λ^*) of the Euler–Lagrange equation $DF(u^*) = \lambda^*$, where $\lambda^* \in \mathbb{R}^m$ denote Lagrange multipliers. We define the free energy $F(u) = \Phi(u) + \Psi(u)$ of the distribution u as the sum of the strongly convex *segmentation entropy*

$$\Phi(u) = \int_\Omega \varphi(u(x))\,dx, \quad \varphi(u) = \sum_{i=0}^m u_i \log(u_i), \tag{4}$$

and of the *nonlocal interaction energy*

$$\Psi(u) = \frac{1}{2}\int_\Omega \sum_{i=0}^m (Ku)_i(x)\,u_i(x)\,dx, \quad (Ku)_i(x) = \int_\Omega \sum_{\ell=0}^m k_{i\ell}(x,y)\,u_\ell(y)\,dy. \tag{5}$$

Note that the logarithmic potential φ in (4) reflects the Fermi-type behavior of the particles. To control the behavior of nonlocal interaction between particles of type i and $\ell \in \{0,\dots,m\}$, we introduce matrix kernels $(k_{i\ell})$ that ensure that particles of the same type attract and particles of different type repel each other. This leads to the desired phase separation. For the sake of numerical simplicity, we use in our applications Green's functions of elliptic Neumann boundary value problems as elements of the matrix kernel: According to (5), we define $(Ku)_i$ as the solution to the problem

$$\begin{cases} -r^2\nabla\cdot\nabla(Ku)_i + (Ku)_i = \sum_{\ell=0}^m \sigma_{i\ell}u_\ell & \text{in } \Omega, \\ \nu\cdot\nabla(Ku)_i = 0 & \text{on } \partial\Omega. \end{cases} \tag{6}$$

Here, we prescribe effective ranges $r > 0$ and intensities $\sigma_{i\ell} \in \mathbb{R}$ of interaction forces between particles of type i and $\ell \in \{0,\dots,m\}$, respectively. The cases $\sigma_{i\ell} > 0$ and $\sigma_{i\ell} < 0$ represent repulsive and attractive interaction, respectively.

In many applications, one is mainly interested in u^*. However, F is, in general, not convex, so it is difficult to solve the Euler–Lagrange equation directly. One possible remedy is to construct u^* as steady state of the evolution system (1): In view of the fact that the Lagrange multipliers λ_i^* should be constant, one assumes their antigradients to be driving forces towards equilibrium. This leads to the evolution system (1), with current densities $j_i = -\sum_{\ell=1}^m a_{i\ell}(u)\nabla\lambda_\ell$, potentials $\lambda_\ell = D_\ell F(u)$, and positively semidefinite *mobility* matrices $(a_{i\ell})$; see [3], [4]. If all of the particles have the same diffusive properties, the hydrodynamical limit process yields mobilities $a(u)$ that are given by the inverse Hesse matrix $(D^2\Phi(u))^{-1}$. In [4], we have shown unique solvability and regularity properties of the evolution system (1). In addition to that, we have developed a dissipative discretization scheme with respect to space and time; see [1]. Figure 3 shows numerical results for a two-component phase separation process in a square with a spatial discretization of 1,024 by 1,024 pixels.

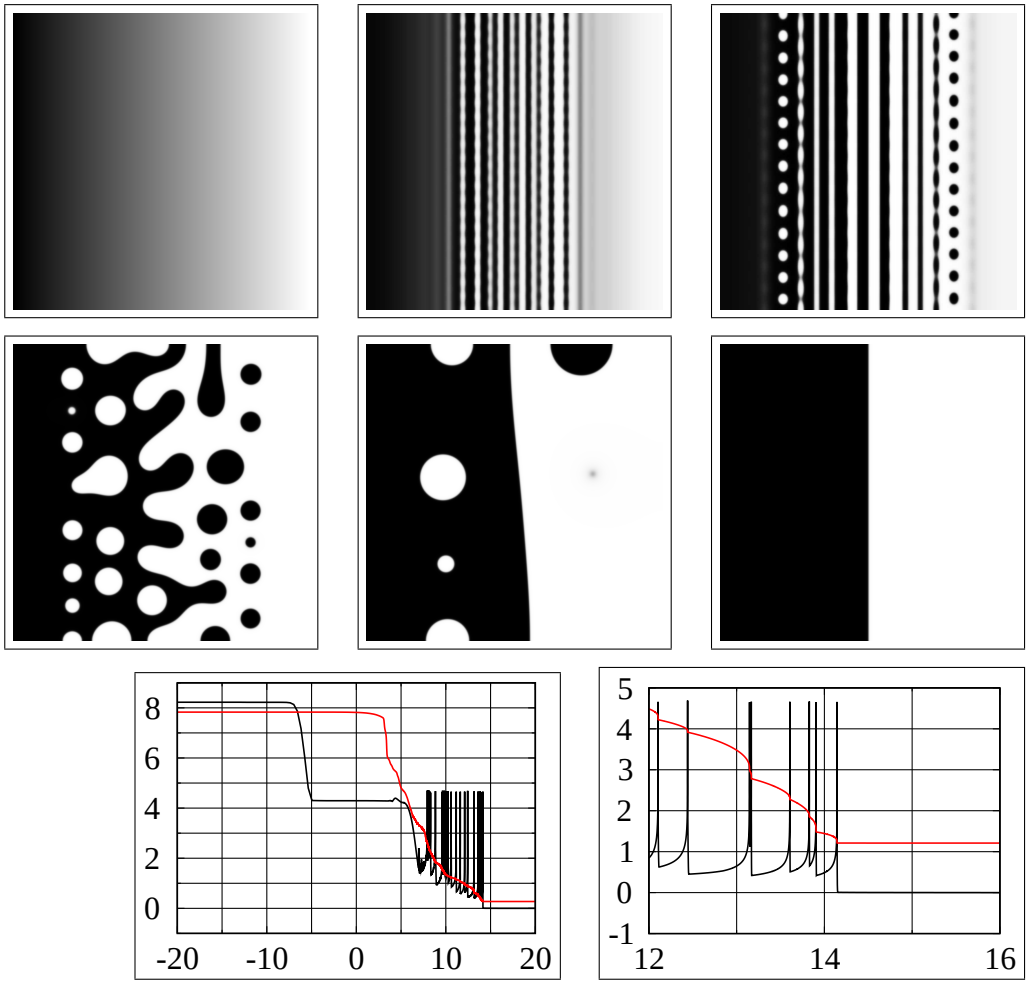

Fig. 3: *Phase separation process in a binary system: (a) Initial value, black to white ramp; (b) formation of stripes; (c) accumulation of balls; (d) unification to coarse structures; (e) nearly final state, death of all the smaller structures; (f) final state, both phases separated by a straight line; (g) decay of the free energy (red line) and evolution of the maximal modulus of λ (black line) along the trajectory on a logarithmic time scale; (h) the same quantities near the end of the simulation.*

However, from a practical point of view this approach becomes questionable if metastable states occur, while one is only interested in the final state u^*. For this purpose, we have developed a descent method, which yields a sequence of intermediate states (u^k) converging to some steady state u^*; see [2]. We minimize the free energy $F = \Phi + \Psi$ of the multicomponent system under the constraint of mass conservation, using the following recursively defined descent method: Let $\tau \in (0, 1]$ be some suitably chosen relaxation parameter and let u^0 denote the initial distribution. Knowing the intermediate state u^k, we uniquely determine v^k and the corresponding Lagrange multiplier $\lambda^k \in \mathbb{R}^m$ by solving an auxiliary problem with a strongly monotone operator:

$$\lambda^k = D\Phi(v^k) + D\Psi(u^k), \quad \int_\Omega v^k(x)\,dx = \int_\Omega u^0(x)\,dx. \tag{7}$$

Finally, we set

$$u^{k+1} = \tau v^k + (1-\tau)u^k. \tag{8}$$

In [2], we have shown that in the limit $k \to \infty$ the sequence (u^k, λ^k) converges to a solution (u^*, λ^*)

of the Euler–Lagrange equation

$$\lambda^* = D\Phi(u^*) + D\Psi(u^*), \quad \int_\Omega u^*(x)\,dx = \int_\Omega u^0(x)\,dx. \tag{9}$$

Simultaneously, the sequence $(F(u^k))$ of free energies decreases monotonically to the limit $F(u^*)$.

Figure 4 shows simulation results for two very similar initial values in a square with a spatial discretization of 256 by 256 pixels. Both initial configurations contain equal numbers of black, white, and medium gray particles, respectively. Obviously, the final states do not only depend on these integral quantities.

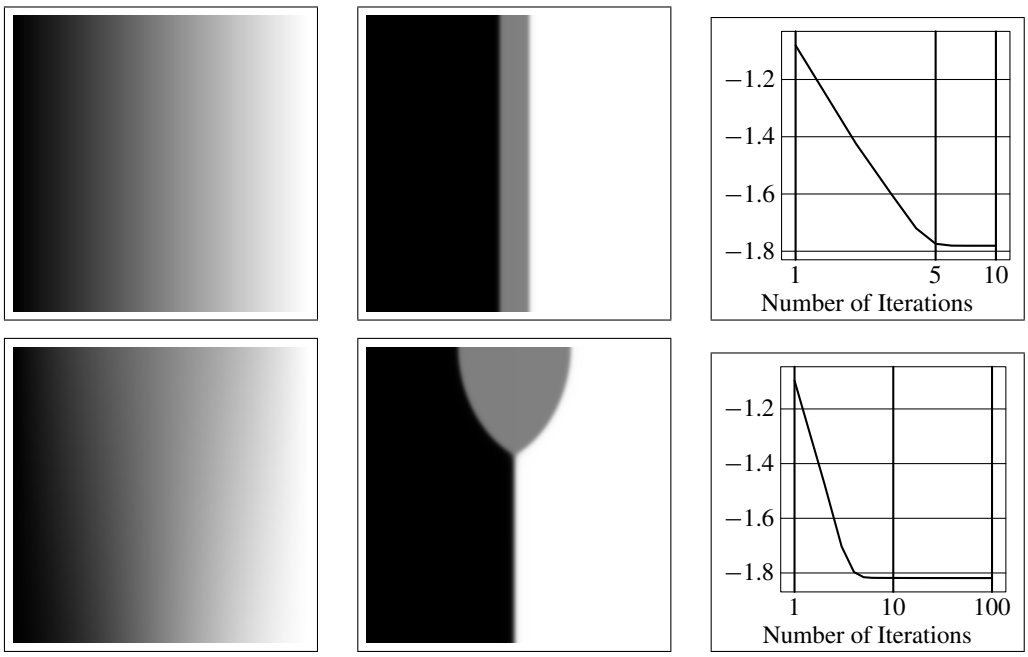

Fig. 4: *Phase separation processes in a ternary system: (a) Initial value, constant in vertical direction; (b) final state, stripe pattern; (c) decay of the free energy to the corresponding local minimum; (d) slightly distorted initial value; (e) final state, phases separated by two arcs and a straight line; (f) decay of the free energy to the global minimum.*

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2.6 Spatially Adaptive Analysis of fMRI Experiments

Jörg Polzehl and Karsten Tabelow

The analysis of *functional Magnetic Resonance Imaging (fMRI)* experiments has been the topic of several WIAS Colloquia. The problems presented there, and our discussions with the lecturers afterwards formed the starting point for our interest in this field. At approximately the same time, we established first results on adaptive smoothing methods that seemed useful in this context. In the last years, research has been carried out in collaboration with several partners, starting with F. Kruggel (Max-Planck-Institut für Kognitive Neurowissenschaften, Leipzig) and F. Godtliebsen (University of Tromsœ, Norway), to name two of them. Currently our main collaborators are H. Voss (Citigroup Biomedical Imaging Center, Weill Medical College, Cornell University) and I. Wartenburger (Berlin Neuroimaging Center, Charité). Our research interests have broadened and now also include *Diffusion Tensor Imaging (DTI)* and other medical imaging techniques. Research on fMRI is essentially carried out within the project *Image and signal processing in medicine and biosciences (A3)* in the DFG Research Center MATHEON.

Let us shortly explain what fMRI is and where statistics comes in when fMRI data is to be analyzed. FMRI is a non-invasive tool for studying the functionality of the brain and for localizing cognitive functions. It has become more and more important in the last few years and is now used not only in neurosciences, but also for such applications as presurgery planning. Activation in the brain is not subject to direct measurement. Instead, the *Blood Oxygenation Level Dependent (BOLD) effect* is used as a natural contrast in fMRI experiments to detect neural activity [5]. The data is obtained as a time series of three-dimensional (3D) images and is characterized by a high noise level and a very low signal-to-noise ratio. The spatial resolution (voxel size) is typically of the order of 3–4 mm. The length T of the time series usually is between 100 to 1,000 scans, with a repetition time of 2 or 3 seconds. The data is correlated in space and time. Figure 1 illustrates a fMRI data set from a right-hand finger-tapping experiment.

The three-dimensional images are recorded while the patient has to perform one or several tasks, like finger tipping, or has to respond to some acoustic or visual signal (stimulus) in a designed experiment. The neural activity associated with this tasks causes, with some time delay, an increased oxygen demand at some locations in the brain. This effect can be measured due to the oxygen-level-dependent magnetic properties of blood (BOLD effect). The regions where an increase in the oxygen level is observed are of interest.

We adopt the common view of a linear model

$$Y_{it} = X_t \beta_i + \epsilon_{it} \tag{1}$$

for the time series $Y = (Y_t)_{t=1,\dots,T}$ in each voxel i, [3]. The X_t specifies the *expected BOLD response* $x(t)$ at time t for each experimental stimulus, and additional effects to model mean level and drift. The noise ϵ_{it} is correlated in time, due to the short acquisition times. The parameter vector β_i is to be estimated in all voxels i. Let $\gamma = c^T \beta$ denote a component of β that corresponds to the experimental stimuli or a contrast between such components.

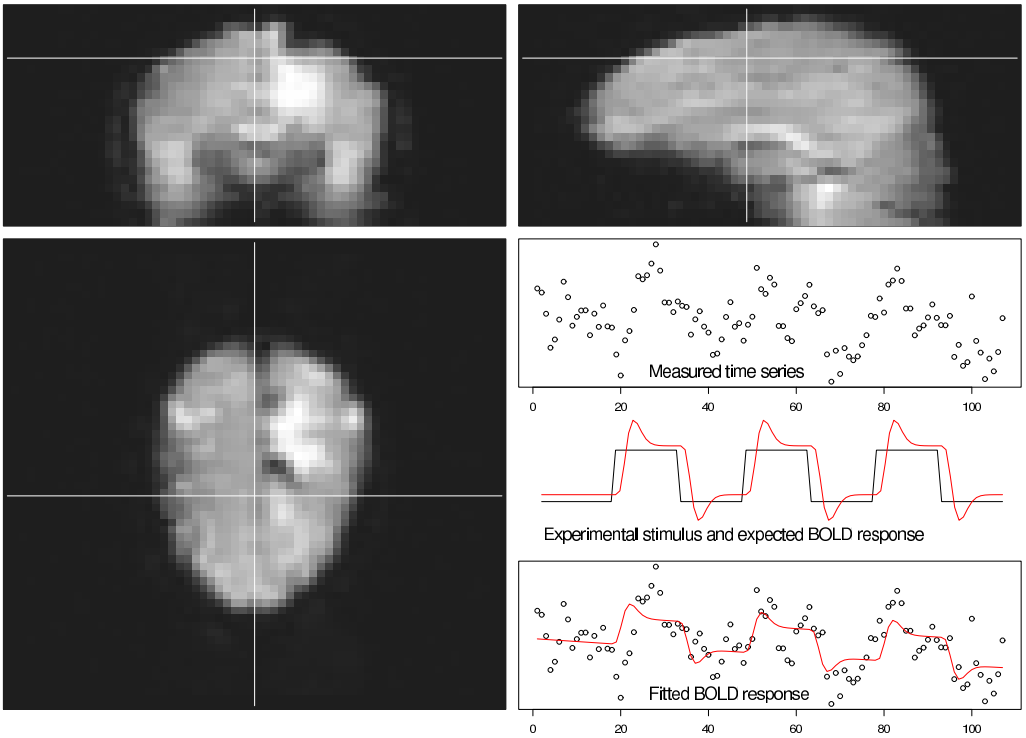

Fig. 1: *Illustration of fMRI data from a right-hand finger-tapping experiment. The figure shows horizontal and vertical slices, intersecting in one voxel i, of the 3D image observed at the first time point. The lower right panel presents the time series observed at this point. Additionally, the stimulus function $s(t)$ and the expected BOLD response $x(t)$ are displayed. Data: H. Voss, Cornell University.*

The estimates of γ form a three-dimensional parameter array. A decision whether a voxel i shows neural activity connected with the experimental stimuli can now be made based on the properties of this array. In voxels without or with unrelated neural activity, we expect the corresponding value in our parameter array to vary around zero. In case of neural activation, the expected value will be different from zero. Therefore we could, in each voxel, test the hypothesis $H_i : \gamma_i = 0$ against an alternative $A_i : \gamma_i \neq 0$. This induces a severe multiple test problem. A typical 3D image in fMRI consists of about 100,000 voxels. A voxelwise analysis using individual critical values at a significance level of $\alpha = 0.05$ therefore produces about 5,000 false positive signals. This is in contrast to some hundreds of activated voxels we are looking for. Additionally, voxels carrying a small signal may be concealed due to high variability of the estimated parameters. The use of a global critical value, i.e., the specification of an error probability to observe a false positive in any voxel, usually leads to no signal detection at all. One solution is to smooth the parameter array. This reduces variability, while the mean value is preserved in spatially extended regions with similar values of γ. At the same time, a correlation structure is induced in the parameter field that allows for much lower global thresholds.

Polzehl and Spokoiny [1] suggested a smoothing procedure called *adaptive weights smoothing (AWS)*. In contrast to other approaches, this technique adapts to different sizes and shapes of objects in the images rather than over-smoothing them. Theoretical results for a generalized approach have been obtained in [6]. In [2], the use of AWS for signal detection in fMRI experiments has been suggested. This paper left several questions open. The approach was restricted to periodic activations, it did not consider temporal and spatial correlation present in the data, and finally, it failed to provide a formal solution to select appropriate thresholds for signal detection.

We are now ready to answer these questions and provide a broad approach for using structural adaptive smoothing in a general analysis of fMRI data. This is discussed in detail in [7]. Here, we provide a short overview.

In contrast to common practice, we start with a voxelwise analysis of the time series in order to get a sufficient dimension reduction prior to spatial smoothing. In case of nonadaptive smoothing, this does not significantly change the results of the analysis.

Voxelwise analysis

The expected BOLD response can be modeled by a convolution of the experimental stimulus with the *hemodynamic response function (HRF)*. This function has been measured and models the fact that, although neural activation is thought to be practically instantaneous to the stimulus, blood oxygenation is subject to some delay. For a stimulus $s(t)$, defined as 1 at task time and 0 at rest, we arrive at the expected BOLD response as a convolution of $s(t)$ and $h(t)$. The resulting function $x(t)$ and the experimental stimulus of a right-hand finger-tapping experiment are illustrated in Figure 1. We create a BOLD signal for each experimental stimulus (usually one or two), and consider the linear model (1) with the first components of X_t chosen as the value of the expected BOLD signal at time t, i.e., as $x(t)$. The first components of β therefore correspond to the stimuli used in the experiment.

The estimation of the parameter β is done separately in each voxel. In order to access the variability of the estimates β correctly, we have to take the correlation structure of the errors ϵ within the time series into account. We here follow [3] assuming an AR(1) model. The autocorrelation coefficient and error variance are estimated from residuals. A bias correction is applied to correct for correlation caused by fitting the linear model. We then use prewhitening to transform (1) into a linear model with approximately independent errors. Finally, estimates of $\gamma = c^T\beta$ and Var $\hat{\gamma}$ are obtained in the prewhitened model.

Spatial smoothing and signal detection

We now arrange the estimates of γ obtained in each voxel and their estimated standard deviations in three-dimensional arrays $\mathcal{G}$ and $\mathcal{S}$. The voxelwise quotient of both arrays $\mathcal{T} = \mathcal{G}/\mathcal{S}$ forms a *statistical parametric map (SPM)*. What we have obtained is approximately a random t-field, see, e.g., [4], with a correlation structure induced by the spatial correlation present in the fMRI data. This correlation structure can be estimated from the residuals in the prewhitened linear model.

Signal detection is now performed by calculating the excursion sets of the SPM $\mathcal{T}$ employing an appropriate global threshold. The geometry of random fields provides an elegant way to obtain such thresholds. For a random t-field, it was shown in [4] that the p-value for its maximum Z, i.e., the probability $\mathbf{P}(\mathbf{Z} \geq \mathbf{z})$ to exceed a threshold z, can be approximated by the expected *Euler Characteristic (EC)*. The expected EC essentially depends on the size of the search volume and the spatial correlation in the t-field $\mathcal{T}$.

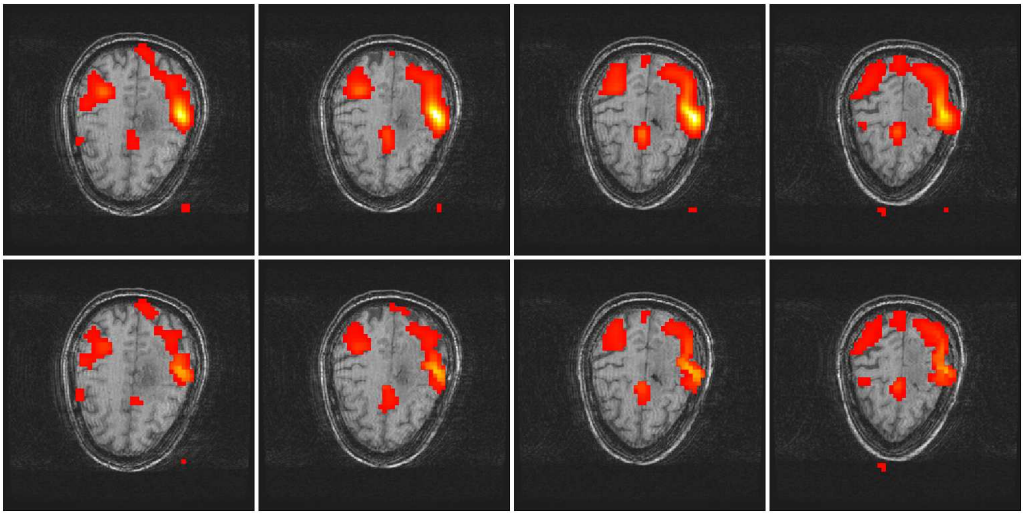

Fig. 2: *Signal detection for the fMRI data illustrated in Figure 1. Slices 17–20. Upper row: nonadaptive smoothing with bandwidth (FHWM) $h = 13.2$ mm, Lower row: adaptive smoothing with maximal bandwidth (FHWM) $h = 13.2$ mm.*

Signal detection based on the original data, using a global threshold that reflects the spatial correlation inherent in the data, only shows very large signals. Nonadaptive spatial smoothing leads to a reduction in variance, while the signal is averaged over spatially extended activations. We therefore observe an increase of the values in the t-field obtained from the smoothed signal in such activated voxels. At the same time, increased spatial correlation leads to a smaller number of independent resolution elements (*resel counts*) and therefore lower global thresholds. This comes at the cost of loss of spatial information at the border of activated regions.

Spatially adaptive smoothing [6] avoids this drawback by restricting the averaging to regions of homogeneity in the data. We use a three-dimensional AWS algorithm that allows for spatially heteroscedastic variances. The procedure uses a Gaussian kernel for localization in space and can be viewed as a direct generalization of the nonadaptive spatial smoothing procedure commonly applied in fMRI analyses. Parameters in this procedure are selected by a propagation condition (see [6]) that ensures that the algorithm behaves like a corresponding nonadaptive smoothing algorithm in large homogeneous regions. In the statistical map $\mathcal{G}$, the largest homogeneous region is formed by voxels in areas not related to the experiments, while smaller regions correspond to areas of activation that are characterized by values of γ different from zero. Therefore, under the hypothesis $H : \gamma = 0$, the AWS procedure approximately behaves like the nonadaptive smoothing procedure, and again the expected EC can be used to obtain approximate global thresholds for the random t-field obtained from smoothing $\mathcal{G}$. The separation property of AWS allows to clearly separate activated areas from regions that are not affected by the experiment.

Figure 2 illustrates the different results obtained by nonadaptive (top row) and spatially adaptive smoothing (lower row) for four consecutive slices. Significance of signal detection is coded by colors ranging from red (at threshold) to white (zero p-value).

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2.7 The Block Oriented Process Simulator BOP

Jürgen Borchardt, Dietmar Horn, and Peter Mathé

Introduction

Many processes in very different industrial plants can be mathematically modeled by the same type of system equations. The numerical solution of these usually high-dimensional systems is called *process simulation*. Over the past three decades, numerical process simulation has become an indispensable tool for the design, analysis, and operation in industrial process engineering. Here, the simulation is used as an "experiment on the model", which is much cheaper, faster, and safer than to perform practical experiments. In this way, it enables to improve the efficiency, safety, reliability, and environmental compatibility of industrial processes.

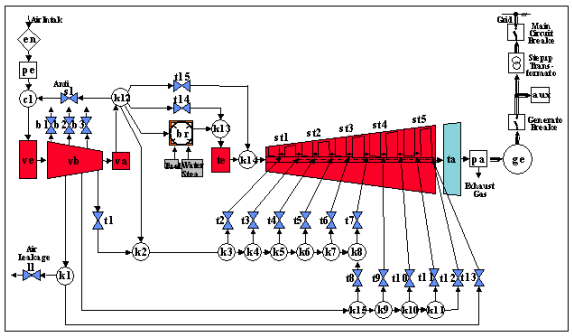

Fig. 1: *Modular model of a gas turbine (ALSTOM (Switzerland) Ltd.)*

Due to an improved accuracy of mathematical process models and an increasing degree of integration in process modeling, the size of the problems that have to be solved numerically has grown considerably. The complex process models used in various process industries depend on numerous parameters, are usually highly nonlinear, and involve discontinuities. Using concentrated physical models, high-dimensional systems of nonlinear and differential–algebraic equations (DAEs) have to be solved in steady-state and dynamic process simulation. For this purpose, robust, reliable, and efficient numerical simulation tools are needed, and the application of parallel numerical methods becomes a challenging task.

Our **B**lock **O**riented **P**rocess simulator BOP uses a simulation concept that takes advantage of the modular structure of the process, which is defined by the hierarchically modular modeling of unit operations (see, e.g., Figure 1). As a result, the corresponding system of equations is structured into subsystems, which can be exploited to speed up its numerical solution.

Until now, BOP has been successfully used for various industrial applications, e.g., for the simulation of batch/continuous distillation, sewage sludge combustion, or heavy duty gas turbine processes.

The simulation concept

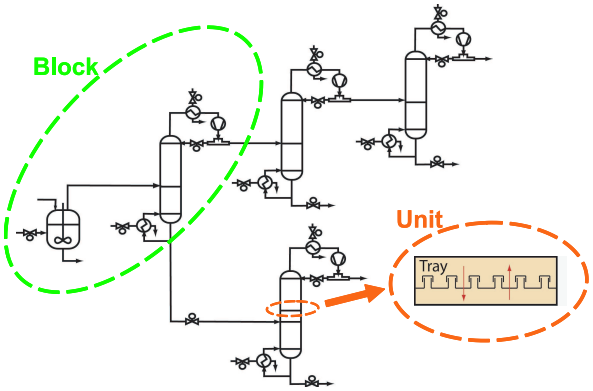

Fig. 2: *Sample of a user-defined block in a part of a reaction-distillation flowsheet*

At WIAS, we have developed a simulation concept for large-scale process simulation that is based on *divide-and-conquer* techniques. In this homogeneous simulation approach, the modular structure of the process is exploited for an efficient numerical solution of the resulting system of equations. Since in most applications the process structure corresponds to the hierarchical unit structure of the underlying plant, the system of equations can be structured into subsystems according to the units. Based on this structure, it can then be portioned into an appropriate number of blocks (see, e.g., Figure 2). This block partitioning can either be predefined by the user or can be generated by different partitioning algorithms. To exploit this hierarchical structure of the system of equations during its numerical solution, we have considerably modified and adapted the standard methods BDF, Newton, and sparse Gaussian elimination.

If the initial value problem for the block partitioned DAE system, which is of the form

$$F_j(t, Y_j(t), \dot{Y}_j(t), U_j(t), \dot{U}_j(t), u(t)) = 0, \quad j = 1(1)p,$$

$$F_j : \mathbb{R} \times \mathbb{R}^{m_j} \times \mathbb{R}^{m_j} \times \mathbb{R}^{n-m_j} \times \mathbb{R}^{n-m_j} \times \mathbb{R}^q \to \mathbb{R}^{m_j}, \quad \sum_{i=1}^{p} m_j = n, \quad t \in [t_0, t_{end}],$$

is solved by implicit integration methods, e.g., using Backward Differentiation Formulas (BDF), then a system of nonlinear equations has to be solved at each discrete point of time. Following the basic ideas in [3] and [4], the corresponding block partitioned system can be appropriately extended to use block-structured Newton-type methods for its solution. These methods use so-called *block Schur complement techniques*.

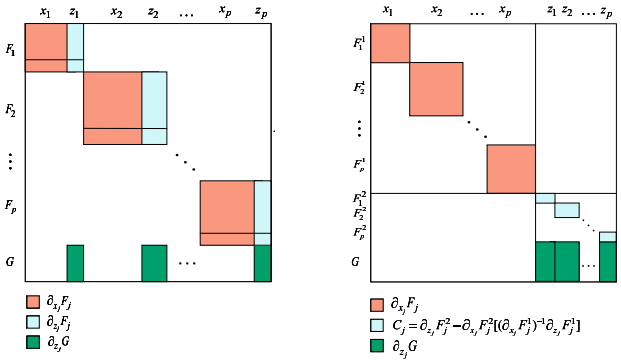

Fig. 3: *Structure of the Jacobian before and after block Schur complement operation*

By the extension, the block functions F_j have disjunctive arguments and the corresponding Jacobian matrix has a special bordered block structure (see Figure 3). This structure is suitable for the application of parallel methods, where the operations on the blocks can be performed concurrently. All calculations for the equation evaluation, the block Schur complement operations, and most of the work needed for the solution of the linear system, can be covered together in one parallel loop. This results in a coarse-grained parallelism, in which the factorization of the coupling matrix (lower matrix in the right part of Figure 3) has turned out to be the main computational bottleneck. To reduce this bottleneck, a controlled relaxation decoupling between blocks has been introduced. In contrast to other methods, this iterative decoupling can be switched off if convergence problems appear.

Monte Carlo simulation

To analyze parameter sensitivities or risk of the simulated process, a Monte Carlo mode has been incorporated into BOP. One major goal of the simulation is to check for optimal adjustment of specified input parameters to guarantee best output. This may be viewed as *sensitivity analysis*.

In case of optimal adjustment of a certain input parameter, small changes of it yield only negligible changes in the output. Thus, locally the input-output relation may be viewed as linear, and the size of the individual input-output correlation will allow to make inference about the adjustment. In statistical terms, this amounts to estimating the *Pearson correlation coefficients*.

The analysis consists of two parts: simulation of the specified input data and statistical analysis of the output data, as well as input-output correlation.

The simulation of the input data is based on triangular distributions for each of the varying input variables. To decrease the variance, *Latin Hypercube* sampling is implemented. The present simulation tools completely cover the capability of previous versions, are however fully integrated into BOP.

The statistical analysis is carried out using the statistical software package **R**. The output data are analyzed under two aspects. First, for each output variable of interest relevant parameters such as mean, and certain quantiles, are estimated and may be displayed graphically. Second, input-output correlations are obtained for each output against each of the input variables. **R** also provides estimates of the 95 % confidence intervals.

The simulator BOP

The sketched simulation concept has been implemented in the **B**lock **O**riented **P**rocess simulator BOP [2]. The simulator uses its own compiler to generate hierarchically structured data and program interfaces from a process description with its high-level modeling language MLPE (**M**odeling **L**anguage for **P**rocess **E**ngineering). This three-stage compiler first analyzes the process description, then links the entire system, and finally generates the data and program interface to the solver of BOP. Each of these phases can be controlled separately. The resulting interface is structured into a unit and a block level, so that the equations can be evaluated independently for units and blocks, respectively. In this way, the compiler has proven to be the key for adapting BOP to industrial needs, because it can transport information about specific features of the model to the interface of the solver, making the simulation process faster and more efficient. In addition to process descriptions using its own language MLPE, the compiler of BOP can also interpret process descriptions that have been written using a subset of the modeling language of the Aspen Custom Modeler™ (ACM)[1] (Aspentech, 2005), one of the most commonly used modeling languages. This renders the simulator usable for a large number of already existing process descriptions in industry.

Main features of BOP are:

- Equation-based modular process description with user-defined procedures
- Steady-state, dynamic, and Monte Carlo simulation modes
- Modified backward differentiation formulas (BDF)
- Block-structured Newton-type methods with controlled relaxation techniques
- Linear sparse matrix solver with partial pivoting and code generation for fast refactorization as well as solution of systems with multiple right-hand sides
- Efficient Jacobian evaluation with combined automatic and numerical differentiation as well as Broyden update techniques
- Setting free variables fixed, and vice versa, without recompiling
- Possible communication with a graphical user interface (GUI) via the Java Native Interface (JNI)

The simulator enables both a classical process simulation for non-structured systems on sequential computers, as well as a concurrent process simulation of block-structured systems on parallel computers with shared memory. Thus, while especially tailored for treating large-scale steady-state and dynamic simulation problems, it can also be efficiently applied to small and medium size problems.

BOP is currently implemented on different shared memory computers using multiprocessing compiler directives (OpenMP) for parallelization. A sequential version for personal computers also runs under Windows and Linux.

[1] see www.aspentech.com

Industrial applications

Up to now, BOP has been successfully used for the simulation of many steady-state and dynamic processes from very different areas. Depending on the different modeling approaches, the resulting simulation problems were of different size and had different numerical properties.

Industrial processes simulated with BOP have been:

1994–2000 Different large-scale batch and continuous distillation processes (*Bayer AG, Leverkusen*)

1999–2000 Sewage sludge combustion process (*Berliner Wasserwerke/Berlin Water Works*)

2000–2001 Catalytic CO oxidation in automotive oxygen sensors (*Bosch GmbH, Stuttgart*)

2002–2005 Industrial gas turbine processes (*ALSTOM Switzerland Ltd., Baden*)

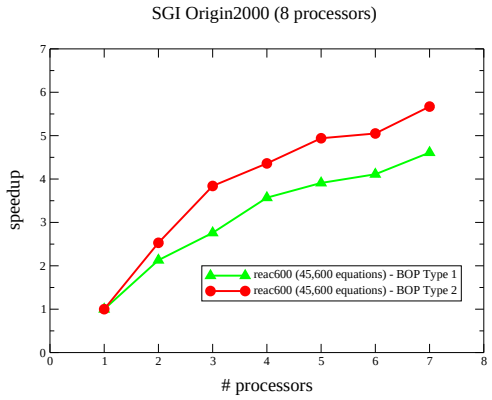

Fig. 4: *BOP: Speedup of overall dynamic simulation runs for a reaction-distillation process*

In this context, BOP has proven to be numerically stable, reliable, and fast. It can be used on both sequential and parallel computers. While the sequential approach is preferable for small- and medium-scale problems, the parallel approach may be used for large-scale problems, e.g., in plantwide dynamic process simulation.

The large-scale problems resulting from plantwide dynamic process simulation of industrial distillation plants have turned out to be a main challenge for our block oriented *divide-and-conquer* strategy and its realization on parallel computers. Figure 4 shows the speedup of overall dynamic simulation runs for a sample process, comparing two different approaches. Practically, these results mean that a process engineer has to wait only about twenty minutes for the simulation result if he uses the block oriented simulation approach of BOP with six processors, compared to more than two hours in the standard sequential case on a single processor. Additionally, we found that for large-scale applications the block oriented *divide-and-conquer* simulation approach can gain speedup factors larger than two, even if it is used in sequential mode on a single processor.

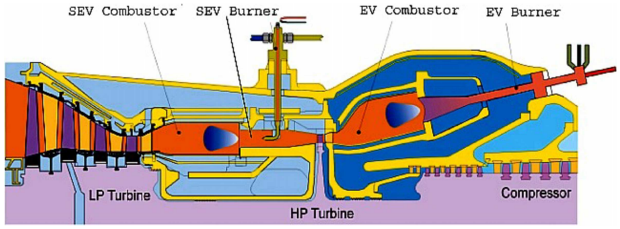

Fig. 5: *Gas turbine for power stations (source: www.power.alstom.com)*

During the last years, the simulator has been adapted to industrial gas turbine simulation. In co-operation with ALSTOM (Switzerland) Ltd., a leading producer of heavy duty gas turbines, we have developed BOP into a simulation package that suits industrial needs.

ALSTOM has developed a new generation of advanced gas turbines (Figure 5), which is used in modern gas-fired combined-cycle power stations. These turbines are based on the so-called sequential combustion technology. In this technology, fuel is injected in the exhaust of the first EV combustor (environmental combustor) of the gas turbine, to initiate a sequential second combustion process. With this technique, capacity and efficiency are increased without increasing the fire temperature. Power augmentation can be achieved, e.g., by inlet cooling and high fogging. The processes that proceed within these turbines are highly integrated, resulting into complex and highly nonlinear process models, which turned out to be the main challenge for the numerical simulation in this application.

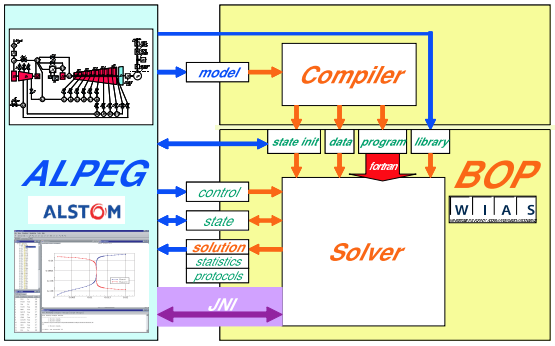

Fig. 6: *Interface ALPEG – BOP*

Based on license agreements, BOP Version 2.1 is being used by ALSTOM for the steady-state process simulation of their heavy duty industrial gas turbines. It runs under the Windows XP operating system on PCs, where it is called up by ALSTOM's graphical user interface ALPEG. Compared to former versions, BOP 2.1 has a number of new features. Among other things, it enables the change of the status of variables from free to fixed and vice versa, without the necessity to recompile and link a new executable. Also, we have implemented changes in the control strategy of the steady-state solver of BOP to improve its reliability and performance even in critical regions of the modeling, as for the problem of anti-icing and the problem of discontinuous modeling with respect to the turbine operation at low part load. Competitive simulation runs for these critical problems have shown that BOP still converges in many cases in which the Aspen Custom Modeler™ (ACM), a worldwide leading commercial simulation tool of Aspen Technology (USA), does not converge. Also, for this application, simulations with BOP perform about three times faster than those using ACM.

The combination ALPEG-BOP is now in successful business use, whereas different versions of this simulation tool can be used by process designers or sales managers, respectively.

In BOP Version 2.2, which is currently under development, the scope of the process description possibilities has been considerably extended, and a Monte Carlo simulation mode has been included. The new simulation mode enables probabilistic statements about the process, as, e.g., probability curves for main performance quantities of the gas turbine process as engine power, engine efficiency, or engine exhaust energy, and its sensitivity with respect to critical process parameters. The Monte Carlo simulation is completely integrated in the simulation concept of BOP. This has proven to be up to one order of magnitude faster than the external Monte Carlo simulation approach used by ALSTOM in the past. This is remarkable, because for a reliable Monte Carlo simulation usually several ten thousands up to some one hundred thousand sample simulations are necessary, implying a large amount of computing time, which is often many hours.

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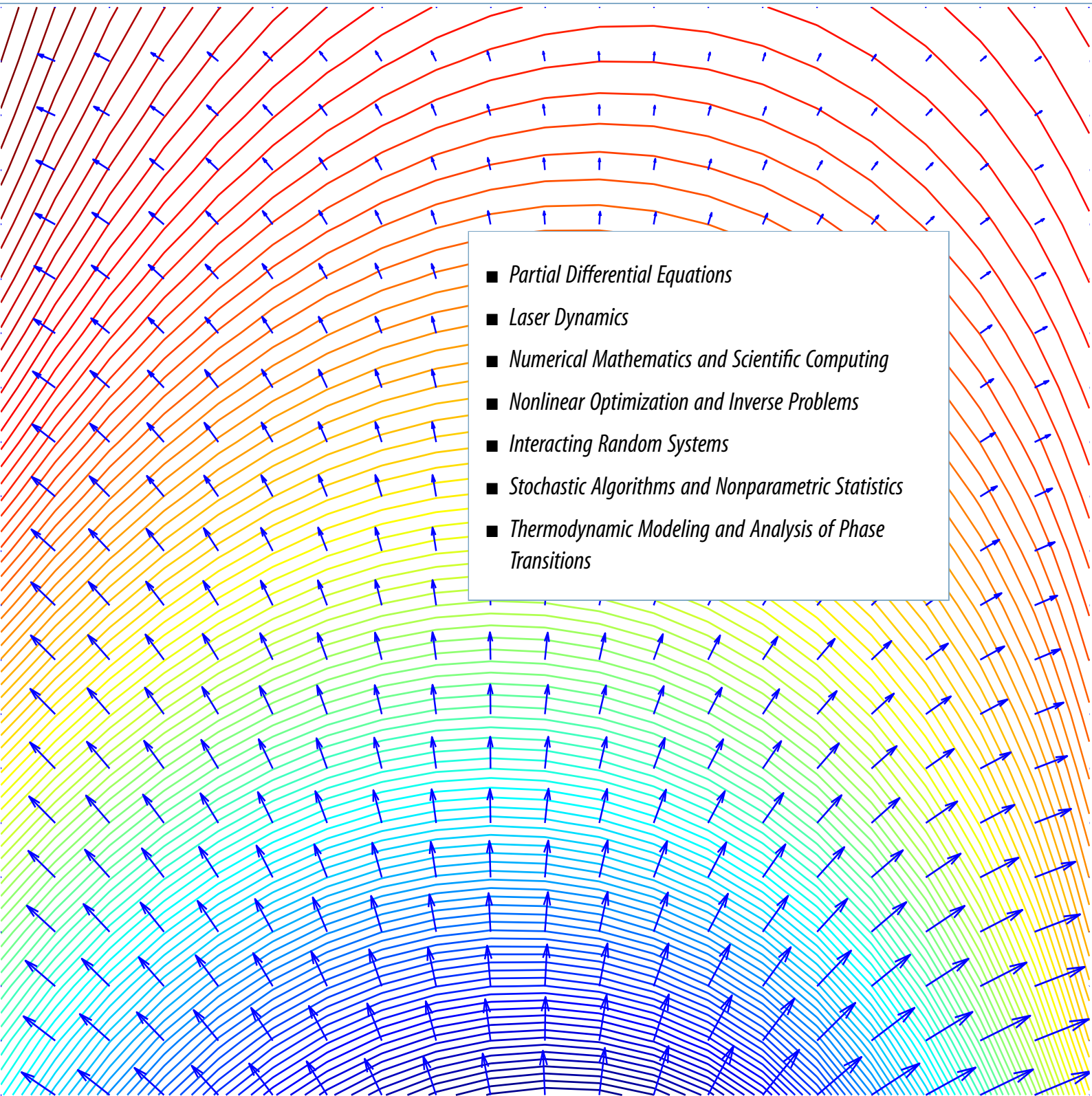
3 Research Groups Essentials



- *Partial Differential Equations*
- *Laser Dynamics*
- *Numerical Mathematics and Scientific Computing*
- *Nonlinear Optimization and Inverse Problems*
- *Interacting Random Systems*
- *Stochastic Algorithms and Nonparametric Statistics*
- *Thermodynamic Modeling and Analysis of Phase Transitions*

3.1 Research Group *Partial Differential Equations*

This research group has undergone some changes since its former head Prof. H. Gajewski retired in 2004 and the new head Prof. A. Mielke took over in early 2005. Moreover, Uwe Bandelow left the research group to become the new head of the Research Group *Laser Dynamics*, taking with him two of his collaborators in the field of optical pulse propagation. Nevertheless, the main focus of the research on applications of the theory of nonlinear partial differential equations remained unchanged. However, the new head established new research topics like material modeling for multifunctional materials and multiscale problems. The main research topics are now:

1. Evolutionary systems with nonlocal interactions, in particular, with applications in semiconductor device modeling and in phase separation problems
2. Modeling of optoelectronic devices including quantum effects
3. Multifunctional materials

The mathematical methods originate from the field of *applied analysis* and range from modeling to analysis and numerical methods. The study of the well-posedness of the underlying partial differential equations leads to a deeper understanding of the underlying physics and provides basic information for the construction of efficient numerical algorithms. In cooperation with other research groups, corresponding software tools are under development that will enable parameter studies or optimization of technological products. The most important mathematical techniques in this research group include:

1. Existence, uniqueness and regularity theory for initial and boundary value problems in nonsmooth domains and with nonsmooth coefficients
2. Coupling of different models, in particular, using models accounting for nonlocal interactions
3. Iterative and variational methods using energetic formulations that are based on physically motivated functionals
4. Qualitative methods for evolutionary systems
5. Multiscale methods for the derivation of effective models on larger scales from models on smaller scales

The modeling of semiconductor and optoelectronical devices constitutes the most active area of the research group. It is done in close collaboration with other applied research institutes and also with industrial partners. On the one hand, the ongoing progress of industrial semiconductor device technologies permits to fabricate devices involving active zones in smaller and smaller sizes; hence, these devices can employ quantum phenomena in their operation, e.g., nanotransistors, tunneling diodes, quantum-well lasers. On the other hand, one is interested in modeling high-energy devices, which can still be modeled on the classical level. In both cases, new physical effects occur that need both, mathematical modeling and numerical simulation.

The worldwide used software package `WIAS-TeSCA` developed by the group is used in several projects at WIAS. A particularly challenging application takes place in a collaboration with the Research Group *Numerical Mathematics and Scientific Computing* and the Semiconductor Laboratory

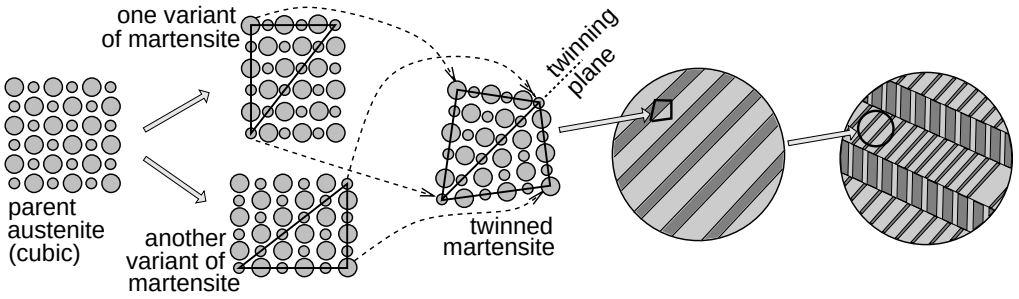
of the Max Planck Institutes for Physics in Munich. The simulations promoted the development of new advanced silicon photodetectors used in high-energy astroparticle physics. The model selection box of `WIAS-TeSCA` has been extended to meet the needs of the associated avalanche processes. Further applications of `WIAS-TeSCA` involve collaborations with the Max Born Institute (MBI) for Nonlinear Optics and Short Pulse Spectroscopy, Berlin, the Walter Schottky Institute (WSI) at the Technische Universität München and the Fraunhofer-Institut für Nachrichtentechnik Heinrich-Hertz-Institut (HHI), Berlin. For MBI the electronic band structure of InAsSb multi-quantum wells has been calculated, and the results have been used at WSI for producing lasers and photodetectors; see [3].

The cooperation with HHI has been done jointly with the Research Group *Laser Dynamics* and was part of the larger project *diMOLA: Monolithic integrated direct modulated 40 Gb transmitter laser OIEC*. While HHI did experiments, simulations were performed at WIAS to develop a suitable design for the multi-section laser. In particular, the Research Group *Laser Dynamics* used the software package `LDSL-tool` for the longitudinal dynamics to find suitable combinations of active and passive longitudinal sections to obtain a device that can be directly modulated by 40 Gb/s. Using `WIAS-TeSCA`, our research group developed an appropriate transverse two-dimensional structure for the laser. The joint efforts of both research groups helped to improve the effectiveness of the lasers considerably and will lead to new designs of devices.

The modeling of semiconductors leads to many challenging mathematical questions in the analysis of the underlying partial differential equations. On the one hand, the drift-diffusion equations for the electronic components are strongly coupled and highly nonlinear; on the other hand, the effectivity of semiconductor devices relies on designs that involve nonsmooth material properties, i.e., the coefficients in the partial differential equations have jumps along polygonal interfaces. A result of K. Gröger from 1989 roughly states that linear elliptic operators in Lipschitz domains are isomorphisms between the Sobolev spaces $W^{1,p}$ and $W^{-1,p}$ for some $p > 2$. Based on this result, in [2] local existence and uniqueness results in two space dimensions have been established for the nonlinear stationary problem, as well as for the dynamical case under more restrictive assumptions. Moreover, significant progress has been made for the question under which additional conditions the isomorphism property also holds for $p > 3$, where $p = 3$ is the physically relevant space dimension. Counterexamples were found, as well as a broad class of polyhedral domains with suitable boundary and transmission conditions, in which the result holds with some $p > 3$. Based on this, and on further newly derived maximal regularity results, there is now in preparation a sequence of new local existence results for quasilinear parabolic equations. For further details see Section 2.3.

Quantum effects are becoming more and more relevant in modern semiconductor devices, owing to the progressing miniaturization. Within the DFG Research Center MATHEON project *Quantum mechanical and macroscopic models for optoelectronic devices*, Michael Baro defended his PhD thesis in September 2005 with the grade “summa cum laude”, since his work covers an important part of this challenging modern field. The thesis spans the whole area from modeling, deriving a selfconsistent coupling between classical and quantum effects, to a deep analysis of the highly nonlinear partial differential equations, to its numerical implementation, and to a comparison with experimental data; see [1], [3].

With the beginning of Prof. A. Mielke's work in early 2005, new topics were installed in the research group, which are related to multifunctional materials and multiscale modeling. The latter area is funded by DFG within the Priority Program SPP 1095 *Analysis, Modeling and Simulation of Multiscale Problems*, which is coordinated by A. Mielke. Recent progress has been made in the modeling of the evolution of microstructure in shape memory alloys. It is based on the recently developed abstract theory for the *energetic formulation for rate-independent systems*; see [5] for the survey in a chapter of "Handbook of Evolutionary Equations". It was possible to establish, for the first time, a model that allows for the prediction of the evolution of gradient Young measures for phase transformations in CuAlNi; see [4] and Figure 1. This model can be fully analyzed in terms of the existence of solutions and of the convergence of suitable space-time discretizations.



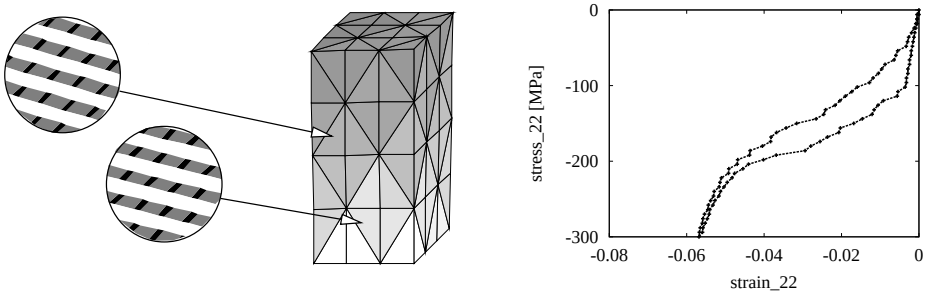


Fig. 1: *Above: Schematic explanation of double-laminate microstructure. Below left: Calculated double laminates under compression. Below right: Calculated stress-strain hysteresis*

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3.2 Research Group *Laser Dynamics*

The research of this group is devoted to the development of mathematical methods and theories in the field of Nonlinear Dynamics, and to applied research projects in optoelectronics. The main topic in 2005 was

Dynamics of multi-section semiconductor lasers.

The research related to this topic includes basic theoretical research on dynamical systems occurring in laser theory, software development, and device simulation. An important contribution to this work consists in the development of the software package `LDSL-tool` for the simulation of spatio-temporal dynamics in complex semiconductor laser devices. This software includes tools for simulation and for numerical bifurcation analysis of a broad class of integrated multi-section or ring lasers. Moreover, the performance of the devices can be analyzed according to the technological requirements in optoelectronic communication systems. The investigations were performed in close cooperation with technology partners and were carried out in the framework of the following projects:

Mode-locking in lasers with saturable absorbers

This project is supported within the research network Terabit Optics Berlin (together with Research Group *Partial Differential Equations*). Using the new modeling approach, which has been developed in the preceeding year ([1]), we were able to perform analytical and numerical investigations of dynamical effects, leading to a degradation of the puls quality in the mode-locked lasers produced by our cooperation partners at the Fraunhofer-Institut für Nachrichtentechnik Heinrich-Hertz-Institut (HHI). By identifying the relevant system parameters, we were able to suggest an improved design of the device where the mode-locking stability range has been substantially increased; see [2].

Numerical methods for laser dynamics

This project is supported by the DFG Research Center MATHEON. The further development of the software package `LDSL-tool` has been focused in 2005 on the following tasks:

(a) Implementation of routines to generate mode approximation systems (ordinary differential equations) and to call the routines of the software tool AUTO for numerical continuation and bifurcation analysis. This allows to calculate and to plot bifurcation diagrams directly from the interface of `LDSL-tool`.

(b) Extension of the software to complex laser configurations, such as multiple coupled ring structures

(c) Implementation of a time-dependent forcing that allows to study the devices under the influence of pseudo-random bit sequence (PRBS) modulations

Together with additional routines for data post-processing and visualization, the additional features of the software have been used for

- Characterization of the signal quality of directly modulated lasers
- Characterization of mode-locking pulsations
- Identification of irregular regimes and estimation of correlation (synchronization) of two unidirectionally coupled chaotic lasers

Dynamics of laser systems with delayed coupling or feedback

The main focus within this project was on systems of delay differential equations with large delay. Using a new theoretical approach (see [3]), we have been able to investigate the instabilities of laser systems with long-delayed feedback and the synchronization behavior of coupled lasers.

In addition, we started to investigate a new type of feedback lasers with resonant feedback from a Fabry–Perot cavity; see [4]. In analogy to the method of time-delayed feedback control, such lasers offer the possibility to stabilize or destabilize lasing states or periodic orbits by the feedback. Research in this project is supported by the DFG Collaborative Research Center 555 “Complex Nonlinear Processes”.

Directly modulated lasers

This project was carried out within the framework of a contract with HHI. The goal of this project was to develop a concept for a new laser device for direct modulation with an electrical data signal at 40 GBit/s. Based on extensive numerical studies, we have been able to suggest a device concept that uses the photon-photon resonance and suppression of relaxation oscillations in feedback lasers to achieve this challenging goal [5]; see Figure 1. The project has been carried out in cooperation with Research Group *Partial Differential Equations*, contributing investigations on the transversal laser design.

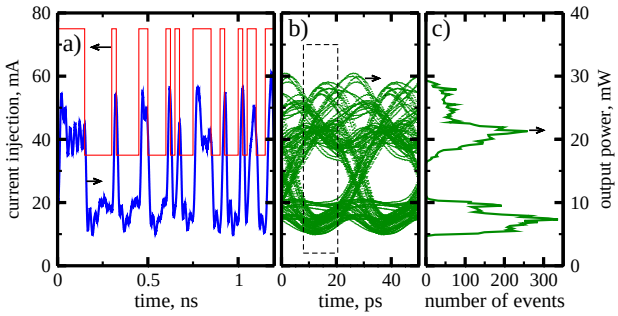

Fig. 1: *Simulated response of the newly developed laser device under PRBS current modulation. (a): injected current (red), field output (blue). (b): open eye diagram. (c): histogram of points within the dashed box of panel (b).*

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3.3 Research Group *Numerical Mathematics and Scientific Computing*

Numerical Methods for Differential Equations

The mathematical description of a significant number of scientific and technological problems leads to *differential equations* that express the relations between temporal and spatial variations of the state of the corresponding physical system.

If the state has no spatial structure, or if the spatial structure can be neglected, systems of *ordinary differential equations* are adequate. In combination with possible additional algebraic equations, they form systems of *differential–algebraic equations (DAEs)*. Among many other problems, electrical networks, and chemical plants, can be modeled using systems of DAEs. If spatial structure comes into play, *partial differential equations (PDE)* are used as models. PDEs describe problems like structural analysis, fluid dynamics, electric and magnetic fields, or diffusing particles.

Typically, problems in science and technology cannot be solved in closed form, and *numerical methods* have to be applied to calculate *approximate solutions*. This process is described in detail for DAEs in Section 2.7, where special emphasis lies on the application to gas turbine simulation. We give a short overview of the algorithms developed by the research group for PDEs and their applications.

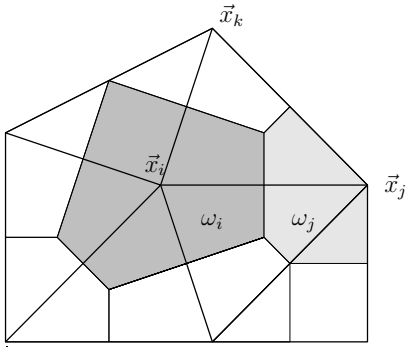

Fig. 1: *A Voronoi box*

The unknowns in PDEs are functions of one or several spatial variables and, possibly, of time. Computers can represent them only approximately. Among several possibilities to generate such approximations, it is the *finite volume method* that lies in the focus of research of the group. This method basically assumes that the computational domain is partitioned into a finite number of *control volumes*, open polygonal boxes around the discretization points, which in some way are similar to representative elementary volumes (REV) used in the derivation of a large class of physical models. Every unknown function is then approximated by its average over the control volume. By integrating the partial differential equation, and using Gauss's theorem, it is possible to calculate the rate of exchange with the neighboring control volumes.

The projects of the group concern a number of theoretical and algorithmical questions related to

this method. At the same time, the finite volume method constitutes the numerical basis of several applied projects. In the following, we give a brief description of several key projects of the research group.

Theoretical investigation of the finite volume method

In cooperation with R. Eymard (Université Marne-la-Vallée), the group studies a finite volume discretization of a wide class of nonlinear convection-diffusion equations. The technique uses a one-dimensional projection of the initial PDE onto the edges connecting neighboring control volumes in order to derive the exchange terms. Stability and convergence of the method have been shown in [1].

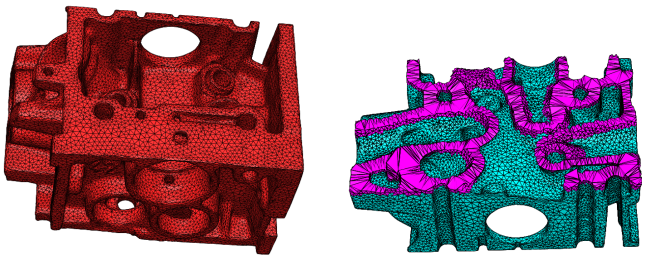

Fig. 2: *Engine part (IFP, France): geometry, TetGen mesh*

TetGen: Tetrahedral grid generation

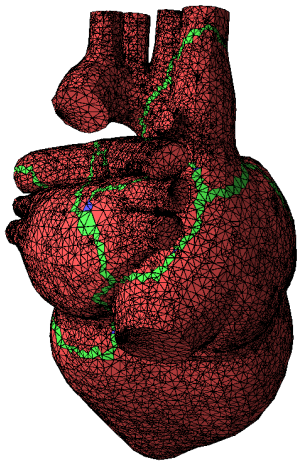

Fig. 3: *Human heart: meshed by TetGen and partitioned*

In order to meet the stability requirements of the method, a suitable approach to gain a partition of a three-dimensional polygonal domain into control volumes starts with a subdivision into tetrahedra. It then suffices to join the midpoints of the circumspheres of the simplices to obtain the *Voronoi boxes* that serve as the control volumes; see Figure 1. order that this procedure be possible, geometrical constraints on the tetrahedral grid have to be imposed. These can be met, provided it complies with the boundary conforming Delaunay property. The development and implementation of algorithms for the generation of such tetrahedral grids lies in the focus of the TetGen project; see [2].

PARDISO: Parallel sparse direct solver

Upon compilation of all equations of exchange between neighboring control volumes, one is left with a large system of linear (or nonlinear) equations, at least as many as control volumes, which count in hundreds of thousands. These systems are *sparse*, i.e., each equation involves only a small number of unknowns. The PARDISO project carried out in cooperation with O. Schenk from the University of Basel, Switzerland, is concerned with the further development of algorithms and software for the numerical solution of such large sparse linear systems, using the well-known

Gauss method tuned in such a way that it runs efficiently on shared-memory parallel computers, [3]. The resulting software is available for a broader public as part of the Intel Math Kernel Library.

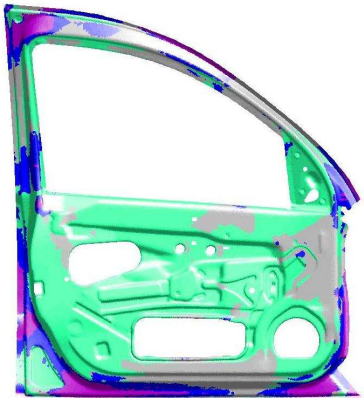

Fig. 4: *Audi-TT door (Autoform): stresses computed using PARDISO*

pdelib2: Software for the numerical solution of PDEs

In the pdelib2 project, a software environment is developed in which all of the above-mentioned components are made available for applied projects. Its data structures are based on multidimensional arrays. These arrays are used to store solutions, grids, matrices, and other objects. The user can directly access the grid generators triangle and TetGen. For parallel computations, the generated grids are partitioned using METIS. The linear algebra subroutines and the programming interfaces for matrix assembly and nonlinear operator application support parallel implementations for shared-memory computers. Various Newton methods for the solution of nonlinear problems are available. The resulting linear problems are solved by iterative and direct solvers. For data description and solution control, a large part of the programming interface has been made accessible from the extension language Lua. The visualization of the computed data may be performed using OpenGL. Finally, graphical user interfaces for specialized problems can be designed using the FLTK toolkit. The pdelib2 environment or various of its components are used within several application projects of WIAS.

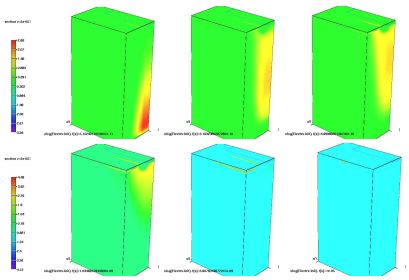

Fig. 5: *DEPFET: an electron cloud moves through the device*

Semiconductor photon detectors

Semiconductor photon detectors are highly sensitive devices using the **DE**pleted **P**-channel **F**ield **E**ffect **T**ransistor (DEPFET) principle in order to integrate a first amplification stage into the photon detector for one pixel. Such detectors are planned to provide the sensor technology for a space-based X-ray telescope. Future digital cameras could profit from such a design as well. In cooperation with R. Richter (Halbleiterlabor, Max-Planck-Institut für extraterrestrische Physik, Munich), a system of three PDEs describing electrostatic potential, electron and hole concentration, is solved in a three-dimensional domain representing a DEPFET sensor cell. The numerical method has to be able to track the charge of less than 100 electrons on its way through the device over time scales ranging from femtoseconds up to seconds. Based on these simulations, the design of the sensor cell has been modified in order to reduce the number of lost photons in the detection process; see [4].

Direct methanol micro fuel cells

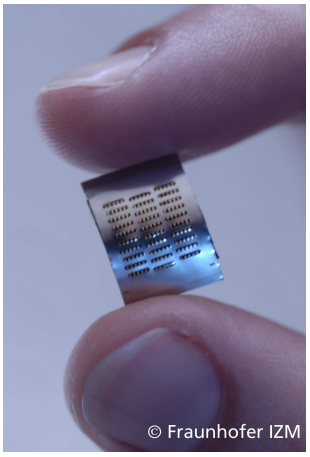

Fig. 6: *Micro fuel cell (Fraunhofer IZM)*

Direct methanol micro fuel cells are possible candidates for replacing rechargeable batteries in cell phones, laptops, and other small devices by a system with a significantly higher capacity. Mathematical and numerical modeling allows for a better understanding of the complex transport and reaction phenomena in such a cell. Based on experience from former projects [5], the research group coordinates the project “Modelling, Experimental Investigation and Numerical Simulation of Direct Methanol Micro Fuel Cells” funded by the German Ministry of Education and Research (BMBF). This project joins several universities and the Fraunhofer Institute for Reliability and Microintegration (IZM), Berlin. At WIAS, starting from an existing numerical model for membrane electrode assemblies of direct methanol fuel cells, simulation models for micro fuel cells and for experimental setups, such as half cells and thin layer cells shall be developed. Special emphasis lies on the modeling of the transport processes within the porous transport layers and the polymer electrolyte membrane, and on the catalytic reaction kinetics.

Thermohaline convection in the subsurface

A possible source for presently observed and historically recorded sources of salt water in the Berlin–Brandenburg region is free convection induced by heated water rising from deeper sedimental layers. This process can be described by a nonlinearily coupled system of three PDEs, describing water flux, heat transport, and transport of salt dissolved in water. In cooperation with the group of Prof. Bayer (GeoForschungsZentrum Potsdam), and supported by the DFG Priority Program SPP 1135 “Dynamics of Sedimentary Systems under Varying Stress Regimes: The Example of the Central European Basin”, comparative simulations using the finite-element-based code FEFLOW of WASY GmbH (Berlin) and the finite volume method described above, have been performed. So far, the results from both codes support the above geological hypothesis; see [6].

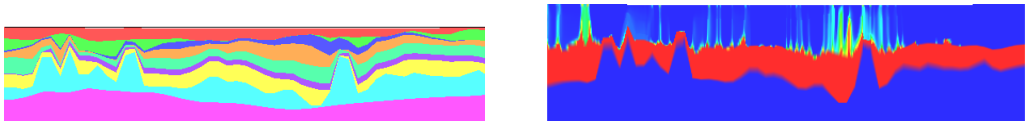

Fig. 7: *Layer structure and salt concentration*

Photoresist development modeling

The technology for creating semiconductor devices includes photolithography, which consists in depositing a photoresist layer on top of a semiconductor wafer, exposing certain parts of it to light, and etching away the exposed (or unexposed) regions. An intermediate step after the exposure is the so-called *post exposure bake*: chemical reactions running at an increased temperature transform an acid distribution created by the light into a distribution of a dissolution inhibitor, which resists the later applied etching agent. In cooperation with A. Erdmann, B. Tollkühn (Fraunhofer Institute of Integrated Systems and Device Technology (IISB), Erlangen), three-dimensional parallel benchmark calculations of this process have been performed. The results are promising, and additional effects will be taken into account in the future, [7].

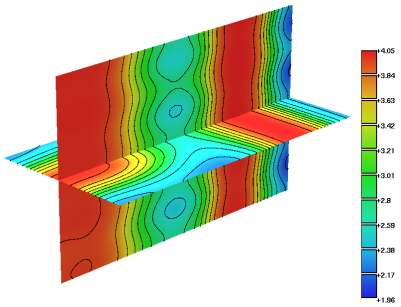

Fig. 8: *Inhibitor concentration for T-structure*

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3.4 Research Group *Nonlinear Optimization and Inverse Problems*

Introduction

The research group studies the optimization of structures and processes, and their interaction. The tasks range from basic research on the formulation, analysis, and numerics of the optimization problems to the development and implementation of efficient numerical algorithms, to the solution of tangible applied problems in cooperation with partners from industry and from the applied sciences. The work is financially supported by industrial partners, BMBF, and DFG.

The strategy of the research group is to engage in long-term cooperations with industrial partners, which are supported by direct industrial money and the joint acquisition of grants. In 2005, the research group has continued their successful work in the fields

- Optimization and inverse problems in diffractive optics and electromagnetics
- Optimal control of production processes

Jointly with E. Uhlmann, TU Berlin, the group has succeeded to acquire an interdisciplinary project related to high-performance milling in the new DFG Priority Program 1180 “Prediction and Manipulation of Interaction between Structure and Process”. In addition, a proposal for a “Specific Targeted Research Project” within the *Sixth EU Framework Programme for Research and Technological Development (FP6)* related to the optimal employment of robots was initiated and coordinated. Although exceeding the threshold in the evaluation process and ending on the list of retained proposals, the application was eventually not funded due to limited EU funds.

A special highlight was the organization of the WIAS Workshop “New Trends in Simulation and Control of PDEs” (September 26–28). Fifty scientists from 13 countries discussed new results related to simulation and control, as well as inverse problems, especially for the Maxwell equations.

The group is collaborating on joint projects with other research groups at WIAS concerning optoelectronic sensors (with Research Group *Partial Differential Equations*), optimal regularity for elliptic and parabolic operators (with Research Group *Partial Differential Equations*), envelope function approximation for electronic states in semiconductor nanostructures (with Research Groups *Partial Differential Equations* and *Numerical Mathematics and Scientific Computing*), and the modeling of phase transitions (with Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*).

Optimization and inverse problems in diffractive optics and electromagnetics

Optical gratings, i.e., periodic surface structures, represent an important class of diffractive elements. They exhibit structural details in a size ranging from a few microns up to a hundred nanometers, and are employed in numerous modern optical devices. For a rigorous simulation, based on Maxwell’s equations, and for the optimal design of general gratings, the FEM package `DiPoG` has

been developed at WIAS in the past years. In 2005 the new version DiPoG-2.1 has been completed, which now provides optimization tools for polygonal grating structures. More precisely, this version is capable of optimizing polygonal interfaces in profile gratings and more general grating structures (simulating, e.g., photolithographic masks).

The objective function can be chosen either as a linear or quadratic expression of the efficiencies and of the phase shifts of the various reflected and transmitted modes of the grating illuminated under different angles of incidence. In contrast to the former version, the case of *conical diffraction* (ray of incident light is oblique to the cross-section plane) is included. The parameters to be optimized include geometric parameters of the grating, like heights, widths, or coordinates of the corners of the polygonal interfaces. Also, the refractive indices of the material components can be optimized.

The optimal design tools of DiPoG include *local* optimization methods based on gradients, such as conjugate gradient and interior point methods, and on the method of augmented Lagrangians. The gradients needed in the optimization algorithms are determined by the finite element method, using the same matrix as for the simulation but different right-hand sides. To avoid problems with local optimal solutions, DiPoG also employs the *global* algorithms of stochastic search and simulated annealing.

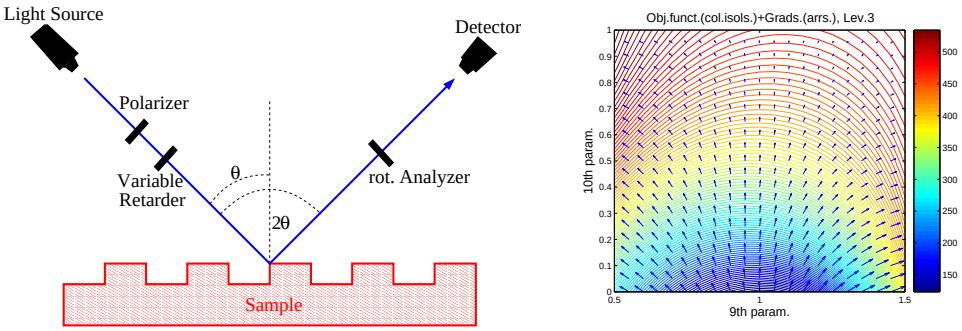

Fig. 1: *Left: draft of scatterometric device, right: isolines and numerically determined gradients of an objective functional w.r.t. two geometry parameters.*

These optimization tools also allow for the reconstruction of geometry parameters in scatterometry. In order to find an efficient reformulation of the reconstruction in terms of optimization problems, the question of uniqueness for inverse diffraction problems has been analyzed from the theoretical point of view. The reconstruction of the shape of periodic structures from measurements of scattered electromagnetic waves is a mathematically challenging inverse problem, owing to the fact that it is both nonlinear and severely ill-posed. In the practically important case of polygonal gratings, new uniqueness results with a minimal number of incident waves were established (cf. [1]).

Moreover, significant progress has been made in the research on the inverse scattering problem of determining a bounded obstacle by its far-field pattern. This problem is fundamental for exploring bodies by acoustic or electromagnetic waves, and its uniqueness has been presenting important and challenging open questions for many years. Uniqueness in the inverse Neumann problem within the class of polygonal domains by a single incoming wave [2] has been shown.

Last, but not least, important progress has also been made in the study of generic shape op-

timization problems subject to elliptic PDE constraints. The convergence of solutions of finite-dimensional auxiliary shape optimization problems to the solution of the original problem has been proven in [4]. Efficient and accurate numerical algorithms have been developed, using BEM or FEM/BEM coupling tools for compactly supported integral objectives (Poisson's equation), with possible applications in fluid dynamics and magnetostatics; see [3]. A proof of compactness of the shape Hessian at optimal (stationary) domains is obtained, implying the exponential ill-posedness of the underlying optimization problems. Both convergence and strict proofs for ill-posedness of compactly supported tracking-type objectives seem to be novel developments in the field of elliptic shape optimization.

Optimal control of production processes

An important approach to modeling risk in engineering applications relies on probabilistic constraints. In 2005, the structure, stability, and numerics of such constraints in the context of optimization problems have been investigated. This is part of project C7 within the DFG Research Center MATHEON, where risk modeling in power production is analyzed. Convexity, compactness, and nontriviality of constraints with stochastic coefficient matrix, have been characterized in [5]. The challenging case of polyhedral chance constraints, where the resulting probability function may fail to be differentiable or even continuous, has been studied in [6]. The main results are an equivalent characterization of continuity and Lipschitz continuity, including a sufficient criterion for differentiability of singular normal distribution functions. In addition, a numerical algorithm for evaluating such functions and their gradients has been derived and tested.

It is foreseen that these results on polyhedral constraints can be utilized also in connection with the optimal control of cooperative robots. According to the demands of the industrial partner, in 2005 the work in this field was centered around three tasks: time-optimal path-planning avoiding collisions, path-planning and simulation of cooperative robots, and a comparison between virtual and real reality, to assure that robotic movements in a virtual shop floor take as long as in reality. An additional challenge in this project is to maintain the real-time capabilities of complete shop-floor simulations including more than 100 active robots and further components.

Coupling with robot path-planning will become important in the near future in MATHEON project C11 regarding the optimal control of laser material treatments. Last year's work in this field concentrated on the analysis and optimal control of thermoelastic models including phase change. By the end of 2005, the new version `WIAS-SHarP2.0` has been released, which uses the new adaptivity concepts realized within `pdelib`. Specific features include the combination of an efficient a priori grid refinement strategy along the moving heat source coupled with a residual error estimator. The biggest success from the applications point of view was the experimental verification of the concept of interplay between machine-based and numerical control in cooperation with *Photon AG*, Berlin. Moreover, by proving exact controllability along a curve for the coupled laser hardening model, also some theoretical justification for the approach [7] could be given.

Finally, a new project has been initiated in 2005 that is concerned with the identification of stable machining conditions for high-speed milling. Here, the goal is a combined modeling of machine, represented by a multi-body system, and process, represented by a thermomechanical model for

the workpiece coupled to an appropriate cutting force model. First results have been obtained for the case of a two-dimensional system with one degree of freedom assuming a rigid workpiece with velocity v_f in the given coordinate system (see Figure 2 (left)). In this case, only the relative movement of the milling cutter with respect to the workpiece has to be considered. Such a simple model can be represented by a two-dimensional ordinary delay differential equation for the displacement of the cutter. The right-hand side of the equation is generated by a cutting force model. The first goal is to carry out a numerical stability analysis that allows to classify the different cutting force models available in the literature. Figure 2 (middle) and (right) shows an unstable milling process, calculated with two different cutting force models.

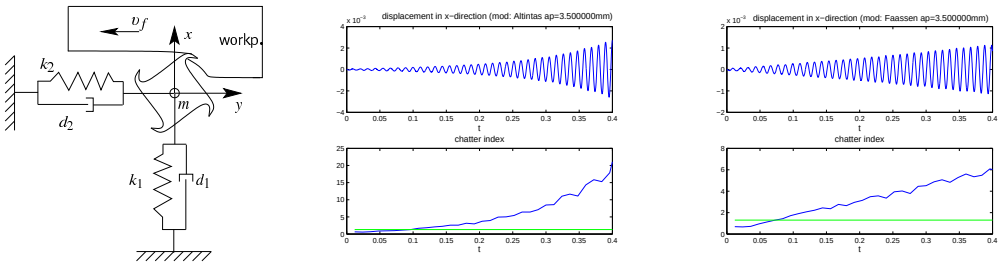

Fig. 2: *Two-dimensional model (left); unstable process – Altintas' model (middle); unstable process – Faassen's model (right)*

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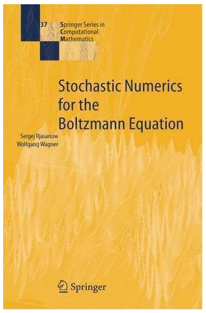
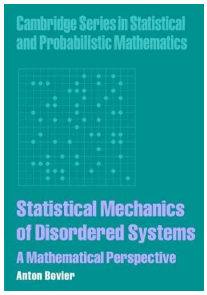
3.5 Research Group *Interacting Random Systems*

The Research Group *Interacting Random Systems* investigates microscopic stochastic models of complex systems arising from a variety of applications in the sciences, economics, and engineering. The main objectives are the rigorous derivation of macroscopic laws, the analysis of long-term behavior, and the development of stochastic numerical algorithms.

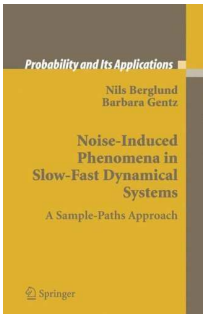
The last year has been a rather eventful one. First of all, three major monographs have appeared or were completed.



Wolfgang Wagner, together with his long-term collaborator Sergej Rjasanow, published "Stochastic Numerics for the Boltzmann Equation" [3], which presents a comprehensive survey of the state of the art in one of the key research themes of our research group. It gives a mathematical description of classical direct simulation Monte Carlo (DSMC) procedures for rarefied gases, using the theory of Markov processes as a unifying framework. Furthermore, it gives a systematic treatment of an extension of DSMC, called stochastic weighted particle method, which is specifically designed for the simulation of rare events.



Anton Bovier wrote "Statistical Mechanics of Disordered Systems" [2], to appear in April 2006 at Cambridge University Press. This book is a graduate-level introduction for mathematicians and for physicists interested in the mathematical foundations of the field, and can be used as a textbook for a two-semester course on mathematical statistical mechanics. The book starts with a concise introduction to statistical mechanics, proceeds to disordered lattice spin systems, and concludes with a presentation of the latest developments in the mathematical understanding of mean-field spin glass models. In particular, recent progress towards a rigorous understanding of the replica symmetry-breaking solutions of the Sherrington–Kirkpatrick spin glass models, due to Guerra, Aizenman–Sims–Starr and Talagrand, is reviewed in some detail.



Barbara Gentz, together with Nils Berglund, wrote the monograph "Noise-Induced Phenomena in Slow–Fast Dynamical Systems: A Sample-Paths Approach" [1], which appeared December 2005 in the Springer Series "Probability and its Applications". This book is a concise account of a research program that aims at developing a constructive approach to the quantitative description of solutions to systems of stochastic differential equations evolving on well-separated time scales. The method, which combines techniques from stochastic analysis and singular perturbation theory, allows the domains of concentration for typical sample paths to be determined, and provides precise estimates on the transition probabilities between these domains. Particular emphasis is put on applications to noise-induced phenomena such as stochastic resonance, hysteresis, excitability, and the reduction of bifurcation delay.

The striking fact that three major monographs have been terminated within the same year shows that the long-term research program our group has been pursuing over the last decade has come to a certain point of maturity in several of its key areas. The considerable body of knowledge that has

been developed through our research warrants a presentation in the form of monographs, which will play an important role in future research on these topics.

A marking event in 2005 was the Les Houches Summer School on Mathematical Statistical Physics, organized by A. Bovier together with F. Dunlop (Université de Cergy-Pontoise, France), F. den Hollander (EURANDOM, the Netherlands), and A. von Enter (University of Groningen, the Netherlands), that took place July 4–28. Funding for the School came from the European Science Foundation, the CNRS (France), the NSF (USA), and the University of Grenoble. Twenty leading scientists of the field presented extended lecture series on the currently most exciting topics at the interface between probability theory and physics, but also on applications in biology, coding theory, and random networks. Fifty-five carefully selected students, both graduate students and postdocs, from around the world were attending the school. Four members of our research group had the chance to participate in this extremely stimulating event. Another major event was a two-week period of concentration on Metastability, Ageing, and Anomalous Diffusion, organized by A. Bovier and St. Müller (MPI-MIS)) at the Max-Planck-Institut für Mathematik in den Naturwissenschaften (MIS-MPG) in Leipzig, May 9–21. This encompassed three series of lectures and a three-day workshop that brought together some of the most active researchers in the field. In the context of the Dutch-German Bilateral Research Group (BRG) "Mathematics of Random Spatial Models from Physics and Biology", a workshop with a focus on stochastic models in biology was organized at WIAS March 16–19. It brought together the members of the BRG and a group of high-level international experts in the field.

A number of major applications for large-scale collaborative research programs were on the 2005 agenda. The application for an International Research Training Group (with Humboldt-Universität Berlin, Technische Universität Berlin, Universität Zürich, ETH Zürich, designated speaker: A. Bovier) received an excellent evaluation from the review panel but was provisionally refused by DFG due to lack of funding; the application was re-submitted this fall. An application for a second three-year funding period of the Bilateral Research Group "Mathematics of Random Spatial Models from Physics and Biology" (DFG/NWO) was submitted. Anton Bovier and Dima Ioffe (Haifa) applied for a research grant with the German-Israeli Foundation (such a grant was approved and became operational for a proposal by Klaus Fleischmann with Achim Klenke (Mainz) and Leonid Mytnik (Haifa)). Finally, A. Bovier was involved in the preparation of a proposal for a Graduate School in Mathematics ("Berlin Mathematical School") that was submitted in the framework of the Excellence Initiative of the German Federal and State Governments by the three universities in Berlin.

Last, but not least, some exciting progress could be made in the research program of the group. We mention the following highlights:

– Essential progress has been made concerning *hydrodynamic limit fluctuations of spatial branching processes with a random catalyst of* ***infinite*** *overall density*. A critical renormalization of mass, time, and space was found that allows to bound random fluctuations asymptotically in both directions by generalized stable Ornstein–Uhlenbeck processes. An interesting new effect is the occurrence of an index jump from a "Gaussian" situation to stable fluctuations of index

$1+\gamma$. Thus, a catalyst with an infinite overall density can have a drastic effect on the fluctuation behavior, and homogenization is no longer the effect governing the macroscopic behavior.

Progress has also been made concerning the limit behavior of rescaled iterates of *renormalization transformations* acting on diffusion matrices of *catalytic* Wright–Fisher diffusions; see [5]. Essential tools are techniques from spatial branching theory as trimmed trees and embedded particle systems in supercritical super-Wright–Fisher diffusions.

– In [6], [7] considerable progress was made in the understanding of the local energy statistics in disordered spin systems. Here one is interested in the spacing and distribution of the realized values of the Hamiltonian of a disordered system in the vicinity of a particular energy level. This issue was first brought up by Stephan Mertens in the study of the combinatorial complexity of discrete optimization problems, in particular the number partitioning problem. He later formulated a universality hypothesis that states that in essentially all conventionally studied models of discrete disordered spin systems, the statistics of energy values should be described by the same Poisson point process. In [6] it was shown that this conjecture holds under very mild conditions. In [7] a particular class of examples, the Generalized Random Energy Models, were considered. In this case it was shown that the conjecture fails when very high energy levels are considered. The more complicated processes that take over beyond this threshold were constructed explicitly.

– In [8] explosion criteria for jump processes with an arbitrary locally compact separable metric state space were established. These results are applied to two stochastic coagulation-fragmentation models—the direct simulation model and the mass flow model. In the pure coagulation case, there is almost sure explosion in the mass flow model for arbitrary homogeneous coagulation kernels with exponent bigger than 1. In the case of pure multiple fragmentation with a continuous size space, explosion occurs in both models, provided the total fragmentation rate grows sufficiently fast at zero. However, an example shows that the explosion properties of both models are not equivalent.

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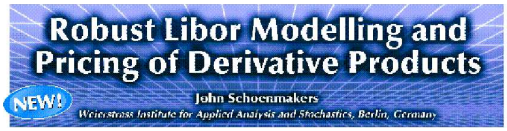
3.6 Research Group *Stochastic Algorithms and Nonparametric Statistics*

The research of the group is organized in the research projects *Statistical data analysis* and *Applied financial mathematics and stochastic simulation*, and focuses on problems from applied stochastics and financial mathematics.

The group's theoretical interests center around topics in applied and algorithmic probability theory and mathematical statistics that include methodological and theoretical aspects of statistical and numerical problems. This is complemented by investigations of their complexity.

The focus is on applications in economics, financial engineering, life sciences, and mathematical physics. Of special interest are the modeling of complex systems using methods from nonparametric statistics, risk assessment, and the valuation in financial markets using efficient stochastic algorithms. The developed methods find applications also in environmental research.

The research group has reached an internationally leading position with important mathematical contributions and the development of statistical software. This is witnessed by the fact that in 2005 the group member M. Reiß has been appointed W3 professor at the University of Heidelberg. As further highlights, two monographs have been written:



J. Schoenmakers published *Robust Libor Modelling and Pricing of Derivative Products* in the Chapman & Hall–CRC series "Financial Mathematics". It includes the latest calibration and pricing methods developed in the research group in the context of the Libor market model. The book was elected into the "Top Ten Finance Books 2005" by the forum "Contingency Analysis".

V. Spokoiny has almost completed his monograph *Local Parametric Methods in Nonparametric Estimation*, to appear in the Springer Series in Statistics.

Part of the research is carried out within three projects in the DFG Research Center MATHEON. Two of them are embedded in *Statistical data analysis*, while the third one is dedicated to applied mathematical finance. Members of the group were involved in several industrial contracts. New pricing methods for Bermudan products have led to a continued cooperation with Bankgesellschaft Berlin AG. In a contract with the Leibniz Institute of Crystal Growth, Berlin, an adaptive smoothing procedure for the online monitoring of crystal mass has been developed and implemented. The group also contributes to the recent version of the **B**lock **O**riented **P**rocess simulator BOP, which is developed in a joint project with ALSTOM (Switzerland) Ltd., Baden. The contribution concentrates on a sensitivity tool, which consists of a Monte Carlo simulation of BOP input and a resulting input-output correlation analysis.

In the following, some scientific highlights achieved by the research group in 2005 are detailed.

Statistical data analysis

Significant progress was made in the theoretical foundation of *structural adaptive smoothing methods*. The new formal concept of *Propagation and Separation* allows for the selection of critical parameters for the different adaptive procedures developed within this project, i.e., adaptive weights smoothing [7], stagewise aggregation, and pointwise adaptive procedures, by a common criterion. This allowed to obtain similar theoretical results for all three types of algorithms. In addition to the local polynomial and one-parameter local likelihood models considered before, the class of models that can be handled by these approaches has been extended to include local generalized linear models. A monograph, [2], is in preparation.

The structural adaptive methods for image denoising are now adapted to allow for more involved image properties, including colored noise and multi-channel images. Image denoising is based on one-parameter local likelihood models and local polynomial models. A first approach to introduce anisotropy in the analysis of two-dimensional images has been successfully tested. A joint application with Y. Schechner (Technion) has been prepared for a research grant on *Adaptive image filtering in attenuating media* with the German-Israeli Foundation.

Essential progress has been made in some exciting applications. Within the project *Image and signal processing in medicine and biosciences* in MATHEON, K. Tabelow and J. Polzehl completed a library for a general analysis of functional magnetic resonance imaging (fMRI) experiments. Open problems like an adequate handling of temporal and spatial correlations are solved, and a formal way for selecting appropriate global thresholds has been obtained; see [8]. The procedures are currently being tested on data provided by our partners from Charité and Cornell University. Incorporation of the tools in established software packages for fMRI (like AFNI or SPM) is anticipated. Further improvements are expected using anisotropic procedures. Work has started on diffusion tensor imaging (DTI) and problems from tomography.

A second project within MATHEON concentrates on *automatic model reduction for complex dynamical systems*. An algorithmic iterative method to estimate the effective dimension reduction (EDR) subspace of real-world stationary molecular systems was developed, which captures their conformational changes. It turned out that this semi-parametric dimension reduction method is able to detect conformational changes in medium-sized oligo-peptides, in good agreement with the computational results for tri- and penta-alanine. The results are reliable even if the conformational changes are rare events on the scale of the complete time series or if the dimension of the state space increases up to 84 in case of B-DNA.

Structural adaptive methods were also successfully applied to the analysis of nonstationary financial time series and dimension reduction problems within a project in the DFG Collaborative Research Center SFB 649.

Applied mathematical finance and stochastic simulation

The central theme of this project is the quantitative treatment of problems raised by industry, based on innovative methods and algorithms developed in accordance with fundamental stochas-

tic principles. The project concentrates on two main areas: *applications in financial industry* and *computational physics*.

As an important scientific result in the *stochastic modeling in finance,* a new iterative method for solving the Bermudan stopping problem, i.e., *pricing of callable derivatives*, was developed, which has led to a major publication [5] and three related subsequent publications. In particular, a scenario selection method has been developed that speeds up this iteration procedure considerably. The method is further extended to complex structured path-dependent interest rate products with call and/or cancellation features. As a practical touchstone, in cooperation with Bankgesellschaft Berlin the valuation of the "cancelable snowball swap" is successfully treated by this iterative procedure. Another approach for American options, based on considering consumption processes developed by D. Belomestny (jointly with G.N. Milstein) in the preceding year, is further enhanced by local analysis of the market. This approach admits the construction of an upper bound (lower bound) of the true price using some lower bound (upper bound) of it. In a diffusion setting, numerical evaluation and hedging of financial derivatives is tackled via Backward Stochastic Differential Equations (BSDEs). A numerical forward scheme for BSDEs is introduced and analyzed by C. Bender (jointly with R. Denk) [3], to approximate prices and hedges for financial derivatives. The method applies to European and American options in unconstrained and constrained markets.
For various interest rate derivatives, the Libor rate model and its calibration is of main importance. The method developed by M. Reiß and D. Belomestny in 2004 on the calibration of the classical exponential Lévy model for an asset price is being extended to a *jump-diffusion Libor market model*, providing a generalization of the calibration procedure for a standard Libor market model in [1]. In the present literature, there is no useful calibration procedure for jump-diffusion Libor models. This research, which has made considerable progress and is still developing, is therefore regarded as a challenge.

In the field of *stochastic models and algorithms in computational physics*, a new *multiscale resolution random field simulation* method has been developed, [6]. It is based on a stratified sampling technique for the spectral representation and a wavelet expansion. This method was applied for random flow simulation in porous media, in turbulence modeling in canopies, and in problems of sound propagation generated by turbulence. This work has been done in cooperation with five international groups, in the framework of the NATO Linkage Grant 981426. An *efficient stochastic numerical method* for the simulation of multicomponent coagulating systems with strongly varying kernels was developed, [4]. This innovative method is applied to the important practical problem of faceted island formation in a crystal growth process, known as Lifschitz–Slyozov–Wagner process, where we have found a new growth regime. This work is carried out jointly with the Paul-Drude-Institut für Festkörperphysik, Berlin.

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3.7 Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*

Overview

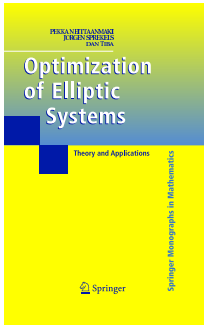
The activities of the research group include multiscale modeling, analysis, and numerical simulations of the dynamics of phase transitions and thin films. The following topics represent the main research areas in 2005.

- Numerical simulation and control of sublimation growth of semiconductor bulk single crystals
- Diffusion of vacancies and arsenic in semi-insulating GaAs, involving the appearance of unwanted liquid arsenic precipitates
- Numerical simulation and control of rotating liquid metallic melts in a changing magnetic field
- Influence of boundary conditions on the equilibria of coexisting phases and sharp interface limits of phase field equations
- Asymptotic hysteresis patterns in a phase separation problem
- Micro-macro transition via modulation theory
- Dynamics of thin polymer films on a hydrophobic silicon wafer

These topics rely on thermodynamic models of large complexity, because they comprise various couplings of different phenomena, for example, diffusion and mechanical stresses. Thus, there arise involved initial-boundary value problems for systems of field equations.

The interdisciplinarity of the group is best illustrated by listing the highlights of 2005 within the various research areas of the group.

In the field of thermodynamic modeling, a study of the evolution of liquid precipitates in a solid surrounding by a Becker–Döring model, which consists of a coupled infinite system of ordinary differential equations, has revealed that the existing models in the literature contradict the second law of thermodynamics. The reason for the failure of the classical models could be resolved, and the proposed alternative Becker–Döring model [1] is already under mathematical investigation by external groups.



In the field of applied analysis, two important contributions to the literature originated from the group. J. Sprekels finished in collaboration with P. Neittaanmäki and D. Tiba a monograph on *Optimization of Elliptic Systems*, which will appear in Springer Monographs in Mathematics, New York, 2006, [2]. P. Krejčí wrote a fundamental study on *Long Time Behavior of Solutions to Hyperbolic Equations with Hysteresis* for the Handbook of Differential Equations, [3].

In the field of thin films, the strategy of the research group to model and study real-life problems proposed by industrial and experimental partners was intensified in 2005. To this end, a four-day interdisciplinary workshop on *Mathematical Problems in Industry: Process Engineering of Thin Liquid Films* was organized. In this workshop, concrete problems from industry were modeled and

mathematically analyzed. The aim of the workshop was to give industrial partners the chance to aim for innovative solutions and new perspectives for a problem of their interest, with the backing of an interdisciplinary team of expert scientists from universities and research institutes. This concept for a workshop has a long tradition, in particular, in the United Kingdom and in the USA; now it has served also here to encourage collaboration between universities, research institutes, and industry. For example, the (DFG-funded) problem of control of thickness and dynamics of polymer films on rotating vertical disks is under investigation. It has important applications in industrial processes, such as polyethylene terephthalate (PET) reactors, and has proven to be very useful for an industrial problem having been presented at the workshop.

In 2005, the research group has organized two further workshops at WIAS. Among the topics of the workshop *Macroscopic Limits and Modulation Theory for PDEs and Discrete Lattice Models* have been: the formal derivation of macroscopic limit equations from microscopic systems (discrete models and PDEs), small amplitude modulation equations like the complex Ginzburg–Landau equation or the nonlinear Schrödinger equation, Whitham's modulation equation for large-amplitude traveling-waves hyperbolicity and Lax conditions, stability properties in micro- and macro-scale macroscopic energies, and stress-strain relations in large-particle limits, energy transport and pulse propagation in dispersive media.

The workshop on *Dynamics of Phase Transitions* focused on the mathematical modeling of phase transitions, which is a rapidly developing research area. Questions of model stability, computational stability, qualitative and/or long-time behavior of solutions, and numerical simulations are highly relevant for technologies of new materials and of melting/solidification processes. The workshop addressed problems arising from various applications, e.g., to crystal growth, shape memory alloys, thin films, flame propagation, or dynamic behavior of biological tissues. Emphasis was put on mathematical and numerical methods of solving the underlying equations describing moving surfaces, small parameter phase transition models, gradient flows, phase field models, or, for instance, models of Ginzburg–Landau, Navier–Stokes–Korteweg, Becker–Döring type, and others.

Finally, J. Sprekels, jointly with F. Tröltzsch (TU Berlin) and others, has organized a workshop on *Optimal Control of Coupled Systems of PDE* at the Mathematisches Forschungsinstitut Oberwolfach.

In 2005, five positions in the research group were financed by grants, one by a DFG proposal on local and nonlocal phase field models, one by the DFG Priority Program 1095 "Analysis, Modeling, and Simulation of Multiscale Problems", and two by the DFG Research Center MATHEON, dealing with thin film dynamics and crystal growth processes. The fifth position was devoted to a coupling of the flow of heat and matter with time-dependent magnetic fields within the interdisciplinary project Krist$\widetilde{Mag}$, which is funded by the Zukunftsfonds Berlin.

Within WIAS, the research group closely cooperates with other research groups: for instance, with the Research Group *Numerical Mathematics and Scientific Computing* on the numerics of systems of PDEs and on visualization, and with the Research Group *Nonlinear Optimization and Inverse Problems* on phase transitions in solids. Joint studies with the Research Group *Partial Differential Equations* concern nonlocal phase field models and macroscopic limits of discrete lattice models.

Among the numerous collaborations with external partners (i.e., other research institutes, universities, industrial partners) are:

– Theoretical studies on the Becker–Döring system, jointly with the applied analysis group at the Humboldt-Universität zu Berlin, and on the transport of gaseous bubbles in a flowing liquid, jointly with the numerical analysis group at the Otto-von-Guericke-Universität Magdeburg
– Comparison of theoretical simulations with experimental results and their application in crystal growth processes, jointly with the Institute of Crystal Growth in Berlin
– Control and optimization of the dissolution of unwanted precipitates in gallium arsenide (GaAs) wafers, jointly with an industrial producer of semi-insulating GaAs wafers

In addition, the research group plays a considerable part in the DFG Research Center MATHEON and in the Graduate School GRK 1128 “Analysis, Numerics, and Optimization of Multiphase Problems”.

Selected studies in detail

Three examples exhibiting major new results may serve to give insight in the various problems studied and solved within the research group.

The first one concerns an interdisciplinary study on the thermodynamics and applied analysis of *the influence of boundary conditions on phase equilibria*. W. Dreyer and C. Kraus reconsidered the two alternatives to model phase transitions: sharp interface models describe the phase boundary between two coexisting adjacent phases by a sharp interface, while phase field models describe this transition by a region of finite thickness. Both models can be physically modeled independently of each other. However, in case that the interfacial thickness is much smaller than the domain of the bulk phases, a sharp interface limit of the phase field model should exist, such that the resulting limit equations coincide with the equations of the corresponding sharp interface model. During 2005, a systematic study of this topic has been initiated.

The first study addresses the problem of the appropriateness of the chosen boundary condition from the viewpoint of the application of phase field models and sharp interface models to physical and technical processes. In particular, the knowledge of the influence of boundary conditions on the resulting phase equilibria is of crucial importance. It often happens that boundary conditions, which are selected according to a mathematical point of view, are not realized in nature or in technological processes.

A cylinder/piston system at constant and uniform temperature, containing a liquid droplet in a gaseous phase, may serve as an example to illustrate the problem. If the external pressure on the piston is fixed, a droplet cannot approach a stable equilibrium; if its initial radius is smaller than a critical radius, which is determined by temperature and pressure, the droplet will vanish, so that there remains the gas phase in equilibrium. If the process starts with a radius that is larger than the critical radius, exclusively the liquid phase will remain in equilibrium. On the other hand, if the approach to equilibrium runs at constant volume of the cylinder, i.e., with fixed piston, it becomes possible to stabilize a droplet of finite radius in equilibrium.

The mathematical literature on phase transitions prefers time-independent domains, which corresponds to processes at constant volumes. However, physical and technological processes, for example the evolution of clouds, run usually at constant pressure, but not at constant volume.

The existing mathematical literature on rigorous sharp interface limits of the Van der Waals–Cahn–Hilliard equation presents proof techniques that only work for constant domains. In 2005, the group has developed alternative techniques that allow for time-dependent domains. The reasoning is based on energy estimates and uniform convergence results for the density u_ϵ as $\epsilon \to 0$, [4].

In connection with these problems, there appeared the following difficulty: within the sharp interface model, the equilibria of a simple liquid/vapor system are given by two conditions that must hold across the interface; the first condition describes interfacial mechanical equilibrium and relates the pressure difference between the two phases to the mean curvature of the interface, the second condition describes phase equilibrium at the interface and states the continuity of the specific Gibbs free energies of the adjacent phases. A careful study of the existing rigorous sharp interface limits of the Van der Waals–Cahn–Hilliard model has revealed that they end up exclusively with the condition for phase equilibrium, however, the condition for mechanical equilibrium is missing. The reason for this strange fact could be identified, and a strategy was established that yields both conditions at the interface.

The second example, in which important new results could be derived, belongs to the field of applied analysis. P. Krejčí studied *asymptotic hysteresis patterns in a phase separation problem*. A classical two-phase evolution system, which goes back to Frémond and Visintin [C. R. Acad. Sci. Paris, Sér. II, 301 (1985), pp. 1265–1268], governed by the energy conservation law and a relaxation phase dynamics, is considered in a bounded thermodynamically insulated domain. If the specific free energy functional is of double-well/double-obstacle type, an energy barrier has to be overcome when passing from one phase to the other, and the two phases may thus coexist in some nondegenerate temperature interval.

It has been an open question for twenty years whether the solution tends to stabilize for large times, and what possible asymptotic states of the system look like. The classical theory of attractors cannot be applied here, due to the lack of space compactness in the phase relaxation equation, and a Lojasiewicz-type asymptotic argument fails due to the lack of smoothness. The preprint [5] proposes a method for solving this problem. It is based on the observation that the solution develops spontaneously two different time scales as time tends to infinity. The temperature evolution becomes slower and slower, while the microevolution on the unknown phase interface keeps its own characteristic speed. This makes it possible to separate the fast local phase dynamics from the slow global heat dynamics, and to consider them independently of each other. Keeping in mind the global energy conservation and nonnegative entropy production, one can exclude a possible chaotic oscillatory behavior and prove that the temperature becomes asymptotically constant and uniform in space, while the phase parameter converges pointwise in space to some distribution of pure states. More specifically, there exists an asymptotic partition of the body into at most three sharp subdomains (typically not connected, with possibly very singular boundaries) of the two pure phases and possibly one intermediate phase. The latter is unstable, and it is conjectured that it does not occur in generic cases, but this remains still an open problem.

The third example demonstrates new highlights in the area of thin film research. B. Wagner and K. Afanasiev studied *thin polymer films on a hydrophobic silicon wafer*. These films tend to recoil from the substrate in a process that is initiated by the formation of holes. The film thickness is reduced from its initial thickness of typically a few tens to hundreds of nanometers to a residual film

of one nanometer or less. Intermolecular forces dominate at these scales and drive the increase of the dewetted area. The process of dewetting and the emerging patterns have attracted considerable experimental and theoretical research. Nevertheless, many of the experimental observations are not yet well understood. Recently, a family of lubrication models have been developed that are derived from the Navier–Stokes free boundary problem with a Navier slip condition at the interface for different regimes of the slip length, covering no-slip to free slippage (e.g., modeling soap films). The investigation of (intermediate and strong) slip has hence opened up a new era in lubrication models with applications to nanoscopic thin films, and has already had an impact on understanding nanofluidic flow. In the case of strong slippage it is found that, for sufficiently large slip lengths, the spatially oscillating structure of the dewetting rim is replaced by monotonic decay. These results are in very good agreement with physical experiments carried out by the collaborators R. Fetzer and K. Jacobs (Universität des Saarlandes) that could not be explained before; see the recent joint paper [6].

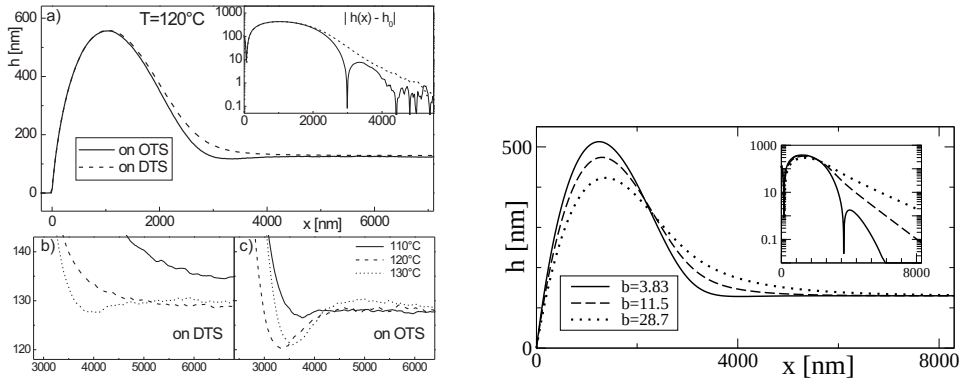


Fig. 1: *OTS covered Si wafers a) at constant temperature (the inset depicts a semilog plot of $|h(x) - H|$), b) and c) at three different temperatures on DTS and OTS surfaces, respectively.* RIGHT: *Rim profiles for different slip lengths b nondimensionalized with $H = 130$ nm. The inset shows a semilog plot of $|h(x) - H|$.*

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[2] P. NEITTAANMÄKI, J. SPREKELS, D. TIBA, *Optimization of Elliptic Systems: Theory and Applications*, Springer Monographs in Mathematics, New York, 2006, 514 p.

[3] P. KREJČÍ, *Chapter 4: Long-time behavior of solutions to hyperbolic equations with hysteresis*, in: Handbook of Differential Equations, Vol. 2: Evolutionary Equations, C.M. Dafermos, E. Feireisl, eds., Elsevier B.V., Amsterdam, 2005, pp. 303–370.

[4] W. DREYER, C. KRAUS, *The sharp interface limit of the stationary Van der Waals–Cahn–Hilliard equation for fixed and for time-dependent domains*, WIAS Preprint in preparation.

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[6] R. FETZER, K. JACOBS, A. MÜNCH, B. WAGNER, T.P. WITELSKI, *New slip regimes and the shape of dewetting thin films*, Phys. Rev. Lett., **95** (2005), pp. 127801/1–127801/4.

A Facts and Figures

(In the sequel the collaborators of WIAS are underlined.)

- Calls, Awards and Distinctions, Habilitations, Ph.D. Theses
- Grants
- Membership in Editorial Boards
- Conferences, Colloquia, and Workshops
- Membership in Organizing Committees of non-WIAS Meetings
- Publications
- Preprints, Reports
- Talks, Posters, and Contributions to Exhibitions
- Visits to other Institutions
- Academic Teaching
- Weierstrass Postdoctoral Fellowship Program
- Visiting Scientists
- Guest Talks
- Software

A.1 Calls, Awards and Distinctions, Habilitations, Ph.D. Theses

A.1.1 Calls

1. M. Reiss, W3 professorship, June 1, Universität Heidelberg, Institut für Mathematik.

A.1.2 Awards and Distinctions

1. Ch. Bender, *Dornier Research Award 2003/04*, July 14.
2. Ch. Kraus, *Award of the "Unterfränkische Gedenkjahrsstiftung für die Wissenschaft" for her doctoral dissertation "On some maximal convergence theorems for real analytic functions in $\mathbb{R}^n$"*, May 11.
3. A. Mielke, *Lecturer Award of Universität Stuttgart for the academic year 2004/05 for his lecture "Analysis III"*, July 1.
4. J. Sprekels, *member of the International Scientific Board of the Institute of Mathematics "Simion Stoilow" of the Romanian Academy, Bucharest.*

A.1.3 Habilitations

1. G. James, *Ondes non linéaires en milieu discrète*, Institut National des Sciences Appliquées, Département GMM, Toulouse, France, supervisor: Prof. Dr. A. Mielke, December 15.

A.1.4 Ph.D. Theses

1. D. Kolyukhin, *Monte Carlo methods for transport simulation in random velocity fields with applications to flow simulation in porous and turbulent media*, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, supervisor: Prof. Dr. K.K. Sabelfeld, November 16.
2. A. Mainik, *A rate-independent model for phase transformations in shape-memory alloys*, Universität Stuttgart, Fachbereich Mathematik, supervisor: Prof. Dr. A. Mielke, January 12.
3. Th. Merkle, *The Cahn–Larché system: A model for spinodal decomposition in eutectic solder*, Universität Stuttgart, Fachbereich Mathematik, supervisor: Prof. Dr. A. Mielke, April 25.
4. M. Baro, *One-dimensional open Schrödinger–Poisson systems*, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. H. Gajewski, September 20.

A.2 Grants[1]

Bundesministerium für Bildung und Forschung (Federal Ministry of Education and Research), Bonn

- **Mathematik für Innovationen in Industrie und Dienstleistungen (Mathematics for innovations in industry and services)**

  "Anwendung eines nichtlokalen Phasenseparationsmodells zur Bildbewertung in der Rheumadiagnostik" (Application of a nonlocal phase separation model to optical diagnosis of rheumatic diseases; in RG 1)

- **Technische Anwendungen der Nichtlinearen Dynamik (Technical applications in nonlinear dynamics)**

  "Hochfrequente Selbstpulsationen in Mehrsektions-Halbleiterlasern: Analysis, Simulation und Optimierung" (High frequency self-pulsations in multi-section semiconductor lasers: Analysis, simulations, and optimization; in RG 2)

- **Netzwerke Grundlagenforschung erneuerbare Energien und rationelle Energieanwendung** (Networks for basic research in renewable energies and efficient energy use)

  "Numerische Simulation für Direktmethanol-Mikrobrennstoffzellen im Verbund MikroDMFC" (joint project on numerical simulation of direct methanol micro fuel cells in the MikroDMFC network; in RG 3)

Deutsche Forschungsgemeinschaft (German Research Foundation), Bonn

- **DFG-Forschungszentrum MATHEON "Mathematik für Schlüsseltechnologien" (DFG Research Center MATHEON "Mathematics for key technologies")**, Technische Universität Berlin

  A3: "Image and signal processing in medicine and biosciences" (in RG 6)

  C1: "Coupled systems of reaction-diffusion equations and application to the numerical solution of direct methanol fuel cell (DMFC) problems" (in RG 3)

  C2: "Efficient simulation of flows in semiconductor melts" (in RG 3)

  C7: "Mean-risk models for electricity portfolio management and stochastic programming" (in RG 4)

  C8: "Shape optimization and control of curved mechanical structures" (in RG 1)

  C9: "Optimal control of sublimation growth of SiC bulk single crystals" (in RG 7)

  C10: "Modelling, asymptotic analysis and numerical simulation of thin liquid films" (in RG 7)

  C11: "Modeling and optimization of phase transitions in steel" (in RG 4)

  D4: "Quantum mechanical and macroscopic models for optoelectronic devices" (in RG 1)

  D8: "Nonlinear dynamical effects in integrated optoelectronic structures" (in RG 2)

  D14: "Nonlocal and nonlinear effects in fiber optics" (in RG 1 and RG 2)

  E1: "Microscopic modelling of complex financial assets" (in RG 5)

  E5: "Statistical and numerical methods in modeling of financial derivatives and valuation of portfolio risk" (in RG 6)

- Collaborative Research Center (SFB) 555, Humboldt-Universität zu Berlin,
  "Komplexe Nichtlineare Prozesse. Analyse — Simulation — Steuerung — Optimierung" (Complex non-linear processes. Analysis — simulation — control — optimization)

  "Analytische und numerische Untersuchungen zur raum-zeitlichen Strukturbildung in Halbleiterlasern" (Analytical and numerical investigations on the spatio-temporal formation of structures in semiconductor lasers; in RG 2)

[1] The research groups (RG) involved in the respective projects are indicated in brackets.

– Collaborative Research Center (SFB) 649, Humboldt-Universität zu Berlin,
"Ökonomisches Risiko" (Economic risk)

B5: "Strukturadaptive Datenanalyse" (Structure-adaptive data analysis; in RG 6)

C4: "Stochastische Optimierung für ökonomische Modelle unter Berücksichtigung von Zeitverzögerungseffekten" (Stochastic optimization for economic models under consideration of time lag effects; in RG 6)

– Priority Program SPP 1095: "Analysis, Modellbildung und Simulation von Mehrskalenproblemen" (Analysis, modeling and simulation of multiscale problems) – Coordinator Program: A. Mielke (in RG 1)

"Elektronische Zustände in Halbleiternanostrukturen und halbklassische Modelle" (Electronic states in semiconductor nanostructures and upscaling to semi-classical models; in RG 1, RG 3, and RG 4)

"Mehrskalenmethoden zur Beschreibung elektronischer Zustände in Halbleiter-Nanostrukturen" (Multiscale methods for the description of electronic states in semiconductor nanostructures; in RG 1, RG 3, and RG 4)

"Mikro-Makro-Übergänge mittels Modulationstheorie" (Micro-macro transitions via modulation theory; in RG 7)

"Makroskopische Dynamik in diskreten Gittern" (Macroscopic dynamics in discrete lattices; in RG 1)

– Priority Program SPP 1114: "Mathematische Methoden der Zeitreihenanalyse und digitalen Bildverarbeitung" (Mathematical methods for time series analysis and digital image processing)

"Structure adaptive smoothing procedures with applications in imaging and functional MRI" (in RG 6)

– Priority Program SPP 1135:"Dynamik sedimentärer Systeme unter wechselnden Spannungsregimen am Beispiel des zentraleuropäischen Beckens" (Dynamics of sedimentary systems under varying stress regimes: The example of the Central European Basin)

"Deep reaching fluid-flow in the Central European Basin System" (in RG 3)

– Priority Program SPP 1180: "Prognose und Beeinflussung der Wechselwirkungen von Strukturen und Prozessen" (Prediction and manipulation of interaction between structure and process)

"Entwicklung eines Prognosetools zur Identifizierung von stabilen Fräsprozessen" (Development of a prognosis tool for the prediction of stable milling processes; in RG 4)

– **Normalverfahren (Individual Grants)**

"Spektralparameterabhängige Randwertprobleme und Hybridmodelle der Halbleitersimulation" (Boundary value problems depending on the spectral parameter and hybrid models in semiconductor simulation; in RG 1)

"Energiemodelle für heterogene Halbleiterstrukturen" (Energy models for heterogeneous semiconductor structures; in RG 1)

"Einfluss räumlicher Fluktuationen auf das Gelationsverhalten von Koagulationsprozessen" (Influence of spatial fluctuations on the gelation behavior of coagulation processes; Technische Universität Ilmenau and in RG 5)

"Hydrodynamische Fluktuationen von Verzweigungsmodellen in katalytischen Medien mit unendlicher Erwartung" (Hydrodynamic fluctuations of branching models in catalytic media with infinite expectations; in RG 5)

"Models for phase transition with thermo-mechanical interaction" (in RG 7)

"Mathematical modeling and analysis of spreading polymer films" (in RG 7)

– Graduate College GRK 251, Technische Universität Berlin
"Stochastische Prozesse und Probabilistische Analysis" (Stochastic processes and probabilistic analysis; in RG 5)

– Graduate College GRK 1128, Humboldt-Universität zu Berlin
"Analysis, Numerics, and Optimization of Multiphase Problems" (in RG 1, RG 3, RG 4, and RG 7)

– In 2005, WIAS hosted a scientist with a Heisenberg fellowship (in RG 7).

– A part of the WIAS guest program was supported by DFG grants.

Alexander von Humboldt-Stiftung (Alexander von Humboldt Foundation)

– 3 scholarship holders (in RG 1, RG 6, and RG 7), see page 140

Deutscher Akademischer Austauschdienst (German Academic Exchange Service), Bonn

– two scholarship holders (in RG 6)

International Projects

– **ESF** (European Science Foundation) Programme "Phase transitions and fluctuation phenomena for random dynamics in spatially extended systems (RDSES)" (in RG 5)

– **EU Research Training Network** "Smart Systems — New materials, adaptive systems and their nonlinearities: Modeling, control and numerical simulation" (in RG 1)

– **GIF** (German-Israeli Foundation for Scientific Research & Development): "Superprocesses and stochastic partial differential equations" (in RG 5)

– **NATO Linkage Grant:** "Stochastic and computational models of transport in porous media" (in RG 6)

– The head of Research Group 5 is a member of the Bilateral Research Group "Mathematics of random spatial models from physics and biology" (DFG/NWO (Netherlands Organization for Scientific Research)), project: "Equilibrium and ageing in glassy systems".

Verbundforschungsvorhaben (research network project): "TerabitOptics Berlin", project B4: "Modellierung und Simulation von Pulsquellen" (Modeling and simulation of pulse sources)

– "Simulation der Pulsausbreitung in nichtlinearen optischen Fasern" (Simulation of pulse propagation in nonlinear optical fibers; in RG 1)

– "Modeling and simulation of mode-locked semiconductor lasers" (in RG 1 and RG 2)

Verbundprojekt (research network project): Krist*Mag* (in RG 7)

Mission-oriented research

– ALSTOM (Switzerland) Ltd., Baden: "Prozesssimulation bei industriellen Gasturbinen" (Process simulation for industrial gas turbines; in RG 3 and RG 6)

– Bankgesellschaft Berlin: "Implementation of the LIBOR market model, calibration and pricing of derivative products" (in RG 6)

– Carl Zeiss AG, Oberkochen: Verbundprojekt/Collaborative project HYBROS (Grundlegende Untersuchungen zu Design und Realisierung neuartiger hybrider Optik-Systeme — basic research into design and implementation of novel hybrid optics systems; in RG 4)

– Fraunhofer-Institut für Nachrichtentechnik Heinrich-Hertz-Institut, Berlin: "diMOLA — Direkt modulierte Laser" (diMOLA — Directly modulated lasers; in RG 1 and RG 2)

- Freiberger Compound Materials GmbH: ”Bildung von As-Ausscheidungen im Spannungsfeld von Versetzungen im GaAs“ (Formation of arsenic precipitates under stresses due to dislocations; in RG 7)
- Freiberger Compound Materials GmbH: “Untersuchung der Evolution einer As-Ausscheidung in GaAs mit einem neu entwickelten Diffusionsmodell zur Erzielung hoher Präzision” (Study of the evolution of a single arsenic precipitate with a newly developed diffusion model that accounts for extremely high precision; in RG 7)
- Institut für Kristallzüchtung, Berlin: “Modellierung und Implementation von Verfahren zum Entrauschen von Messsignalen” (Modeling and implementation of methods to denoise measurement signals; in RG 6)
- Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin: “Berechnung der elektronischen Bandstruktur von InAsSb-Quantenwells” (Calculation of the electronic band structure of InAsSb multi-quantum wells; in RG 1)
- Rücker GmbH, Weingarten: “Simulations- und Optimierungsaufgaben bei der virtuellen Fabrikplanung” (Simulation and optimal control tasks in virtual production planning in automotive industry; in RG 4)
- Volkswagen AG, Wolfsburg: “Modellierung und Parameteridentifikation für Kostenparameter von Fabriken” (Modeling and parameter identification for cost parameters of factories; in RG 4)
- Deutsches Elektronen-Synchronotron (German Electron Synchrotron, DESY), Hamburg: “Risikostudie für die Kostenentwicklung des SFEL-Projekts” (Risk study of the development of the costs in the SFEL project; in RG 5)

A.3 Membership in Editorial Boards

1. A. Bovier, Editorial Board, Markov Processes and Related Fields, Polymat, Moscow, Russia.
2. K. Fleischmann, Editorial Board, Annals of Probability, Institute of Mathematical Statistics, Beachwood, Ohio, USA.
3. R. Henrion, Editorial Board, Journal of Chemometrics, Wiley, New York, USA.
4. P. Krejčí, Editor, Applications of Mathematics, Academy of Sciences of the Czech Republic, Prague.
5. P. Mathé, Editorial Board, Monte Carlo Methods and Applications, VSP, Zeist, The Netherlands.
6. A. Mielke, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
7. ———, Editorial Board, Archive for Rational Mechanics and Analysis, Springer-Verlag, Berlin Heidelberg.
8. ———, Editorial Board, SIAM Journal on Mathematical Analysis, Society for Industial and Applied Mathematics, Philadelphia PA, USA.
9. ———, Editor-in-Chief, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
10. ———, Co-Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
11. ———, Editor-in-Chief, Journal of Nonlinear Science, Springer Science+Business Media, New York, USA.
12. J. Polzehl, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.
13. ———, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, The Netherlands.
14. K.K. Sabelfeld, Editor, Monte Carlo Methods and Applications, VSP, Zeist, The Netherlands.
15. ———, Senior Editor, Mathematics and Computers in Simulation, Elsevier, Amsterdam, The Netherlands.
16. V. Spokoiny, Editorial Board, Annals of Statistics, IMS, Beachwood, Ohio, USA.
17. ———, Editorial Board, Statistics and Decisions, Oldenbourg Wissenschaftsverlag, München.
18. J. Sprekels, Editor, Advances in Mathematical Sciences and Applications, Gakkōtosho, Tokyo, Japan.
19. ———, Editorial Board, Applications of Mathematics, Academy of Sciences of the Czech Republic, Prague.
20. W. Wagner, Editorial Board, Monte Carlo Methods and Applications, VSP, Zeist, The Netherlands.

A.4 Conferences, Colloquia, and Workshops

A.4.1 WIAS Conferences, Colloquia, and Workshops

Workshop Random Spatial Models from Physics and Biology
Berlin, March 16–19
Organized by: WIAS (RG 5)
Supported by: DFG, WIAS

The spring workshop of the Dutch-German Bilateral Research Group on Mathematics of Random Spatial Models from Physics and Biology (co-funded by DFG and NWO), consisting of the groups of A. Bovier (WIAS, RG 5), F. Götze (Bielefeld), A. Greven (Erlangen), F. den Hollander (Eindhoven), and A. Wakolbinger (Frankfurt), was held at WIAS this year. Thematic emphasis this time was on stochastic models related to and inspired by biology. Thanks to additional financial support from WIAS, in addition to the members of the bilateral research group, several international experts working at the interface of probability theory and theoretical biology could be invited, and a lively exchange of ideas among the approximately 35 participants took place. Topics included spatially structured populations, random trees, coalescents and genealogies, branching processes, and random fitness landscapes.

Workshop "Nonlinear Dynamics in Photonics"
Berlin, May 2–4
Organized by: WIAS (RG 1, RG 2), Humboldt-Universität zu Berlin (HU)
Supported by: Technology Foundation Berlin (project "TerabitOptics Berlin"), DFG (SFB 555 "Complex Nonlinear Processes")

The workshop war organized by U. Bandelow, M. Wolfrum (both WIAS), and H.-J. Wünsche (HU). It focused on mathematical, physical, and technological aspects of nonlinear phenomena in semiconductor lasers, optoelectronic devices, and fibers. The main topics included:

– Dynamics of laser systems with coupling or feedback
– Mode-locking and saturable absorbtion
– Nonlinear wave propagation

Following the tradition of preceeding workshops, major attention was paid to an interdisciplinary approach, including the mathematical and physical background as well as technological applications, in particular optical telecommunication technologies. The workshop has been attended by 57 participants from 9 countries, and included 25 invited and contributed talks.

Workshop "Mathematics in Industry"
Berlin, July 18–21
Organized by: WIAS (RG 7), Matheon Project Group C10 "Modelling, asymptotic analysis and numerical simulation of the dynamics of thin film nanostructures on crystal surfaces"
Supported by: DFG Research Center Matheon, WIAS

In the field of thin films, the strategy of the Research Group *Thermodynamic Modeling and Analysis of Phase Transitions* to model and study real-life problems proposed by industrial and experimental partners was intensified in 2005. To this end, a four-day interdisciplinary workshop on *Mathematical Problems in Industry: Process Engineering of Thin Liquid Films* was organized. In this workshop, concrete problems from industry were modeled and mathematically analyzed. The aim of the workshop was to give industrial partners the chance to aim for innovative solutions and new perspectives for a problem of their interest, with the backing of an interdisciplinary team of expert scientists from universities and research institutes. This concept for a workshop

has a long tradition, in particular, in the United Kingdom and in the USA; now it has served also here to encourage collaboration between universities, research institutes, and industry. For example, the (DFG-funded) problem of control of thickness and dynamics of polymer films on rotating vertical disks is under investigation. It has important applications in industrial processes, such as polyethylene terephthalate (PET) reactors, and has proven to be very useful for an industrial problem having been presented at the workshop. The workshop was attended by 32 persons, and 6 talks were given.

5TH INTERNATIONAL CONFERENCE "NUMERICAL SIMULATION OF OPTOELECTRONIC DEVICES" (NUSOD '05)
Berlin, September 19–22
Organized by: WIAS, Humboldt-Universität zu Berlin (HU), Ferdinand-Braun-Institut für Höchstfrequenztechnik (FBH) Berlin
Supported by: HU, FBH, WIAS, IEEE, LEOS, OpTecBB, Berlin Adlershof: City of Science

U. Bandelow of WIAS (then RG 1) was one of the conference's co-chairs. The NUSOD conference was aimed on bridging the gap between theoretical research and practical device development in optoelectronics. Papers have been solicited on the theory, modeling, simulation, and analysis of optoelectronic devices including related materials and applications. 100 researchers, device engineers, and software developers attended the meeting, accompanied by an exhibition of five software companies. On the first day, four tutorials on topics of general interest have been given. The development and the practical use of numerical tools in photonics and electronics have been in the conference's focus.

5TH WORKSHOP "MULTISCALE PROBLEMS IN QUANTUM MECHANICS AND AVERAGING TECHNIQUES"
Berlin, September 22–23
Organized by: WIAS (RG 1)
Supported by: DFG (Priority Program 1095 "Analysis, Modeling and Simulation of Multiscale Problems")

The workshop's organizing committee members were A. Arnold (Technical University of Vienna), A. Jüngel (Universität Mainz), and H.-Chr. Kaiser (WIAS, RG 1). The focus of the workshop was on averaging methods for partial differential equations and multiscale problems arising from the quantum mechanical modeling and simulation of semiconductor nanostructures and their embedding into semiconductor devices. Topics were many-particle systems, quantum-classical coupling, time averages, quantum hydrodynamics, adiabatic and scaling limits, semiconductor nanostructures, electronic structure calculation, upscaling to semi-classical models.

RESEARCH TUTORIAL "RESONANT TRANSPORT IN SEMICONDUCTOR QUANTUM STRUCTURES"
Berlin, September 24
Organized by: WIAS (RG 1), MATHEON Project Group D4 "Quantum mechanical and macroscopic models for optoelectronic devices"
Supported by: DFG Research Center MATHEON

The goal of the research tutorial that was organized by H.-Chr. Kaiser (RG 1) was knowledge raising and interaction of scientists working in mathematics, physics, and engineering on problems which are linked to the same industrial application. The focus of the workshop was on mathematical modeling and numerical simulation of resonant transport in semiconductor quantum structures. We aimed at enhancing cooperation within MATHEON and with the Joint Lab of the Innovations for High Performance Microelectronics GmbH Frankfurt/Oder and the Brandenburg University of Technology Cottbus. The audience comprised applied mathematicians and physicists specialized in condensed matter physics, semiconductor devices, and quantum theory.

WORKSHOP "NEW TRENDS IN SIMULATION AND CONTROL OF PDES" (TISCOPDE05)
Berlin, September 26–28
Organized by: WIAS (RG 4), MATHEON Project Group C11 "Modeling and optimization of phase transitions in

steel"
Supported by: DFG Research Center Matheon, WIAS

Many engineering and scientific problems in design, control, and parameter estimation can be formulated as optimization problems, governed by PDEs. The workshop aimed at bringing together researchers working in numerical analysis, optimal control, and inverse problems of the Maxwell equations and related advanced applications. It was organized by D. Hömberg (RG 4) and J. Sprekels (RG 7) together with F. Tröltzsch (TU Berlin).

The workshop had 51 scientists from 13 countries. Thirty-one talks were presented during the workshop. The contributions covered in particular: scattering theory for rough surfaces and for inhomogeneous media, numerical analysis for eigenvalue problems of the Maxwell equations and for high-dimensional problems with stochastic data, homogenization theory for electromagnetism, efficient preconditioning for large-scale optimization and shape optimization. Interesting applications were presented from interventional cardiology, optimization of induction heat treatment processes, geophysical shape inversion and 3D inverse obstacle scattering problems.

Young Researchers Workshop on Smart Systems
Berlin, October 10–12
Organized by: WIAS (RG 1)
Supported by: European Commission HPRN-CT-2002-00284, WIAS

The Workshop on Smart Systems was organized by A. Timofte (WIAS, RG 1), B. Ayuso (IMATI-CNR Pavia), and L. Beirao da Veiga (Università degli Studi di Milano). Attended by 14 participants from 6 countries, it was intended to improve the direct scientific communication between the Young Researchers in the European Network "New Materials, Adaptive Systems and Their Nonlinearities". It promoted a broader knowledge of the respective research interests between all project units and allowed fruitful discussions and collaborations between researchers working in such different areas like modeling, optimization and control, as well as numerical simulation.

Workshop on Delaunay Grid Generation for Numerical Computations "Tetrahedron"
Berlin, October 13–14
Organized by: WIAS (RG 3)

The Delaunay method is not only one possible method for mesh generation among others, but in many cases, if it succeeds, it yields the "right" meshes for numerical computations. Boundary-conforming Delaunay meshes are essential for finite volume methods. However, there remain serious gaps in the practical realization of this concept. Bridging these gaps, as we believe, is possible only by thorough algorithmical research. The workshop focused on open problems in this direction and on mathematically founded approaches to solve them as, e.g., algorithms for three-dimensional boundary-conforming Delaunay meshes, anisotropic Delaunay meshes, Delaunay meshes in adaptive algorithms. Another focus of the workshop was on application problems, among them groundwater hydrology, liquid crystals, semiconductor devices. The workshop has been attended by 29 participants from France, the United States, and Germany.

Further details can be found at http://www.wias-berlin.de/workshops/tetrahedron.

Workshop on Macroscopic Limits and Modulation Theory for PDEs and Lattice Models
Berlin, November 2–4
Organized by: WIAS (RG 7)
Supported by: DFG (Priority Program 1095 "Analysis, Modeling, and Simulation of Multiscale Problems"), WIAS

Among the topics of the workshop *Macroscopic Limits and Modulation Theory for PDEs and Discrete Lattice Models* have been: the formal derivation of macroscopic limit equations from microscopic systems (discrete models

and PDEs), small amplitude modulation equations like the complex Ginzburg–Landau equation or the nonlinear Schrödinger equation, Whitham's modulation equation for large-amplitude traveling-waves hyperbolicity and Lax conditions, stability properties in micro- and macro-scale macroscopic energies, and stress-strain relations in large-particle limits, energy transport and pulse propagation in dispersive media. The workshop was attended by 41 scientists. Sixteen talks were given.

Festive Colloquium in the Framework of the Langenbach Seminar "Nonlinear Partial Differential Equations"
Berlin, November 9
Organized by: WIAS (RG 1)

This colloquium was organized by the Research Group *Partial Differential Equations* in order to honor the outstanding achievements of Dr. habil. Rolf Hünlich in his scientific vita, who has been one of the organizers of the Langenbach-Seminar for 37 years. The invited speakers were selected among former coworkers and cooperation partners. The talks given focused on the modeling, analysis, and simulation of semiconductor devices, the main area Rolf Hünlich has contributed to for the last two decades. Nearly 60 participants attended the colloquium.

Workshop on Dynamics of Phase Transitions
Berlin, November 30 – December 3
Organized by: WIAS (RG 1, RG 7)

This workshop has focused on the mathematical modeling of phase transitions, which is a rapidly developing research area. Questions of model stability, computational stability, qualitative and/or long-time behavior of solutions, and numerical simulations are highly relevant for technologies of new materials and of melting/solidification processes. The workshop addressed problems arising from various applications, e.g., to crystal growth, shape memory alloys, thin films, flame propagation, or dynamic behavior of biological tissues. Emphasis was put on mathematical and numerical methods of solving the underlying equations describing moving surfaces, small parameter phase transition models, gradient flows, phase field models, or, for instance, models of Ginzburg–Landau, Navier–Stokes–Korteweg, Becker–Döring type, and others. Sixty-six scientists have participated in the workshop. Thirty-two talks were given.

A.4.2 Non-WIAS Conferences, Colloquia, and Workshops co-organized by WIAS and / or having taken place at WIAS

6TH Colloquium of the DFG Priority Program 1095 "Analysis, Modeling and Simulation of Multiscale Problems"
Bonn-Röttgen, June 26–29
Organized by: WIAS (RG 1)
Supported by: DFG

All twenty-two groups of the DFG Priority Program 1095 are meeting annually for exchanging the ideas and methods developed in the past year via a series of about 20 talks. Moreover, in a discussion panel the collaboration for the coming year is planned. The colloquium was organized by the priority program's spokesperson A. Mielke (WIAS, RG 1).

Workshop "Regularity for nonlinear and linear PDEs in nonsmooth domains — Analysis, simulation and application"
Hirschegg (Austria), September 5–7
Organized by: WIAS (RG 1), Universität Stuttgart
Supported by: DFG (SFB 404 "Multifield Problems in Continuum Mechanics)"

The workshop was jointly organized by F. Frehse (Bonn), D. Knees (WIAS, RG 1), and A.-M. Sändig (Stuttgart). Altogether 32 participants from Austria, the Czech Republic, Germany, France, Poland, and Sweden presented regularity results and discussed their numerical treatment for linear and nonlinear elliptic and parabolic boundary and transmission problems on nonsmooth domains. General regularity theory as well as applications in solid and fluid mechanics and piezo-electricity were considered.

A.5 Membership in Organizing Committees of non-WIAS Meetings

1. U. Bandelow, member of the Scientific Committee, *International Workshop on PHysics and Applications of SEmiconductor LASERs (PHASE)*, Metz, France, March 29–30.
2. ———, member of the Scientific Subcommittee, *Conference on Lasers and Electro-Optics/Quantum Electronics & Lasers Science Conference CLEO/QELS 2005*, München, June 12–17.
3. ———, co-chair, *5th International Conference "Numerical Simulation of Optoelectronic Devices" (NUSOD'05)*, Humboldt-Universität zu Berlin, September 19–22.
4. A. Bovier, co-organizer, *Workshop "Metastability, ageing, and anomalous diffusion: Stochastic and nonlinear effects in long term dynamics"*, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, May 9–21.
5. ———, co-organizer, *Summer School "Mathematical Statistical Physics"*, Les Houches, France, July 4–29.
6. Y. Chen, member of the Organizing Committee, *Workshop "Factor Identification in High Dimensional Time Series"*, Berlin, December 9–10.
7. J. Geiser, co-organizer of the Session "Discretisation methods with finite volumes, discontinuous Galerkin methods and the application in porous media, Part I", *Third M.I.T. Conference on Computational Fluid and Solid Mechanics*, Cambridge, USA, June 14–17.
8. ———, co-organizer of the Session "Complex Models in Solid and Fluid Mechanics: Methods and Applications in Multi-physical and Multi-scaling Problems (1–3)", *Eighth U.S. National Congress on Computational Mechanics*, Austin, USA, July 24–28.
9. D. Hömberg, member of the Scientific Committee, *1st International Conference on Distortion Engineering*, Bremen, October 24–26.
10. ———, organizer of the Mini-symposium "Industrial Optimal Control Problems", *SIAM Conference on Mathematics for Industry*, Detroit Marriott Renaissance Center, USA, October 24–26.
11. D. Knees, co-organizer, *Regularity for nonlinear and linear PDEs in nonsmooth domains — Analysis, simulation and application*, Hirschegg, Austria, September 5–7.
12. P. Krejčí, organizer of the Mini-symposium "Rate Independent Processes and Hysteresis", *EQUADIFF 11 International conference on differential equations*, Bratislava, Slovakia, July 25–29.
13. A. Mielke, organizer of the GAMM-SIAM Special Session on Topics in Applied Mathematics, Part D (Multiscale Problems: Oszillations in Partial Differential Equations and Homogenization), *2nd Joint Meeting of AMS, DMV and ÖMG*, Mainz, June 16–19.
14. ———, organizer, 6^{th} *Colloquium of the DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems"*, Bonn–Röttgen, June 26–29.
15. K.K. Sabelfeld, member of the Program Committee, *Vth IMACS Seminar on Monte Carlo Methods (MCM 2005)*, Tallahassee, USA, May 16–20.
16. V. Spokoiny, member of the Organizing Committee, *Workshop "Factor Identification in High Dimensional Time Series"*, Berlin, December 9–10.
17. J. Sprekels, co-organizer, *Workshop "Optimal Control of Coupled Systems of PDE"*, Mathematisches Forschungsinstitut Oberwolfach, April 17–23.
18. ———, member of the Scientific Committee and co-organizer of a focus session, *International Conference "Free Boundary Problems: Theory and Applications"*, Coimbra, Portugal, June 7–12.

19. ———, leader of Breakout Session 5, *DOE Workshop "Transforming Our Energy Future: Advancing The Role Of Science and The Critical Connections With Applied Energy Programs"*, Oak Ridge, TN, USA, November 15–16.
20. B. WAGNER, co-organizer of "The Slippage Session", *Summer Workshop of SPP 1164 "Nano- and Microfluidics: Bridging the Gap between Molecular Motion and Continuum Flow"*, Bad Honnef, August 17–19.
21. W. WAGNER, member of the Scientific Programme Committee, *Workshop on Coagulation-Fragmentation Processes: Theory and Applications*, Edinburgh, UK, July 4–8.
22. ———, member of the Technical Committee, *Workshop "Direct Simulation Monte Carlo: Theory, Methods, and Applications"*, Santa Fe, USA, September 25–28.

A.6 Publications

A.6.1 Monographs

[1] N. Berglund, B. Gentz, *Noise-Induced Phenomena in Slow-Fast Dynamical Systems: A Sample-Paths Approach*, Probability and its Applications, Springer, Berlin, 2005, xiv+276 pages.

[2] J.G.M. Schoenmakers, *Robust Libor Modelling and Pricing of Derivative Products*, Chapman & Hall CRC Press, 2005, 202 pages.

[3] S. Rjasanow, W. Wagner, *Stochastic Numerics for the Boltzmann Equation*, vol. 37 of Springer Series in Computational Mathematics, Springer, Berlin, 2005, xiii+256 pages.

[4] I. Müller, W. Weiss, *Entropy and Energy. A Universal Competition. Interaction of Mechanics and Mathematics*, Springer, 2005, 273 pages.

Monographs (to appear)

[1] A. Bovier, *Statistical Mechanics of Disordered Systems*, Cambridge Series in Statistical and Probabilistic Mathematics, Cambridge University Press, Cambridge.

[2] P. Neittaanmäki, D. Tiba, J. Sprekels, *Optimization of Elliptic Systems: Theory and Applications*, Springer Monographs in Mathematics, Springer, New York.

A.6.2 Editorship of Proceedings

[1] H.-J. Wünsche, J. Piprek, U. Bandelow, H. Wenzel, eds., *Proceedings of the 5th International Conference on "Numerical Simulation of Optoelectronic Devices" (NUSOD '05) in Berlin, September 19–22, 2005*, IEEE, Piscataway, NJ, 2005, 134 pages.

[2] C. Lai, K. Wilmanski, eds., *Surface Waves in Geomechanics: Direct and Inverse Modelling for Soils and Rocks*, vol. 481 of CISM Courses and Lectures, Springer, Wien [u.a.], 2005, v+385 pages.

Proceedings (to appear)

[1] K. Kunisch, G. Leugering, J. Sprekels, F. Tröltzsch, eds., *Control of Coupled Partial Differential Equations. Proceedings of the International Conference in Oberwolfach, April 17–23, 2005*, Intern. Ser. Numer. Math, Birkhäuser Verlag.

[2] P. Colli, N. Kenmochi, J. Sprekels, eds., *Dissipative Models in Phase Transitions. Proceedings of the INdAM Workshop in Cortona, Italy, September 5–11, 2004*.

A.6.3 Outstanding Contributions to Monographs

[1] U. Bandelow, H. Gajewski, R. Hünlich, *Chapter 3: Fabry–Perot Lasers: Thermodynamics-based Modeling, in: Optoelectronic Devices — Advanced Simulation and Analysis*, J. Piprek, ed., Springer, New York, 2005, pp. 63–85.

[2] P. Krejčí, *Chapter 4: Long-time Behaviour of Solutions to Hyperbolic Equations with Hysteresis, in: Handbook of Differential Equations. Vol. 2: Evolutionary Equations*, C. Dafermos, E. Feireisl, eds., Elsevier Science B.V., Amsterdam, 2005, pp. 303–370.

[3] A. Mielke, *Chapter 6: Evolution of Rate-independent Systems, in: Handbook of Differential Equations. Vol. 2: Evolutionary Equations*, C. Dafermos, E. Feireisl, eds., Elsevier Science B.V., Amsterdam, 2005, pp. 461–559.

[4] M. Radziunas, H.-J. Wünsche, *Chapter 5: Multisection Lasers: Longitudinal Modes and Their Dynamics, in: Optoelectronic Devices — Advanced Simulation and Analysis*, J. Piprek, ed., Springer, New York, 2005, pp. 121–150.

A.6.4 Articles in Refereed Journals[2]

[1] B. Jin, A. Acrivos, A. Münch, *The drag-out problem in film coating*, Phys. Fluids, 17 (2005), pp. 103603/1–103603/12.

[2] A. Münch, *Dewetting rates of thin liquid films*, J. Phys.: Condensed Matter, 17 (2005), pp. S309–S318.

[3] A. Münch, P.L. Evans, *Marangoni-driven liquid films rising out of a meniscus onto a nearly-horizontal substrate*, Phys. D, 209 (2005), pp. 164–177.

[4] B. Albers, K. Wilmanski, *Monochromatic surface waves on impermeable boundaries in two-component poroelastic media*, Contin. Mech. Thermodyn., 17 (2005), pp. 269–285.

[5] ———, *On modeling acoustic waves in saturated poroelastic media*, J. Statist. Phys., 131 (2005), pp. 873–996.

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[7] M. Baro, M. Demuth, E. Giere, *Stable continuous spectra for differential operators of arbitrary order*, Anal. Appl. (Singap.), 3 (2005), pp. 223–250.

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[2] Articles that have been written by scholarship holders during their stay at WIAS have been listed in front of those written by the collaborators of WIAS.

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[40] ———, *Transient numerical study of temperature gradients during sublimation growth of SiC: Dependence on apparatus design*, Preprint no. 1080, WIAS, Berlin, 2005.

[41] J. Giannoulis, A. Mielke, *Dispersive evolution of pulses in oscillator chains with general interaction potentials*, Preprint no. 1050, WIAS, Berlin, 2005.

[42] A. Glitzky, R. Hünlich, *Stationary energy models for semiconductor devices with incompletely ionized impurities*, Preprint no. 1001, WIAS, Berlin, 2005.

[43] J.A. Griepentrog, *Local estimates for solutions to generalized heat equations with nonsmooth data*, Preprint no. 1083, WIAS, Berlin, 2005.

[44] ———, *Maximal regularity for nonsmooth parabolic problems in Sobolev–Morrey spaces*, Preprint no. 1084, WIAS, Berlin, 2005.

[45] J.A. Griepentrog, W. Höppner, H.-Chr. Kaiser, J. Rehberg, *A bi-Lipschitz, volume preserving map from the unit ball onto a cube*, Preprint no. 1048, WIAS, Berlin, 2005.

[46] R. Henrion, A. Lewis, A. Seeger, *Distance to uncontrollability for convex processes*, Preprint no. 1059, WIAS, Berlin, 2005.

[47] H. Alder, D. Hömberg, W. Weiss, *Simulationsbasierte Regelung der Laserhärtung von Stahl*, Preprint no. 1085, WIAS, Berlin, 2005.

[48] O. Klein, F. Luterotti, R. Rossi, *Existence and asymptotic analysis of a phase field model for supercooling*, Preprint no. 1042, WIAS, Berlin, 2005.

[49] D. Kolyukhin, K.K. Sabelfeld, *Stochastic flow simulation in 3D porous media*, Preprint no. 1007, WIAS, Berlin, 2005.

[50] Th. Koprucki, M. Baro, U. Bandelow, T.Q. Tien, F. Weik, J.W. Tomm, M. Grau, M.-Ch. Amann, *Electronic structure and optoelectronic properties of strained InAsSb/GaSb multi quantum wells*, Preprint no. 1028, WIAS, Berlin, 2005.

[51] P. Krejčí, S. Zheng, *Pointwise asymptotic convergence of solutions for a phase separation model*, Preprint no. 1055, WIAS, Berlin, 2005.

[52] P. Krejčí, E. Rocca, J. Sprekels, *Nonlocal temperature-dependent phase-field models for non-isothermal phase transitions*, Preprint no. 1006, WIAS, Berlin, 2005.

[53] A. Mielke, *Macroscopic behavior of microscopic oscillations in harmonic lattices via Wigner–Husimi transforms*, Preprint no. 1027, WIAS, Berlin, 2005.

[54] M. Kružík, A. Mielke, T. Roubíček, *Modelling of microstructure and its evolution in shape-memory-alloy single-crystals, in particular in CuAlNi*, Preprint no. 1047, WIAS, Berlin, 2005.

[55] A. Mielke, R. Rossi, *Existence and uniqueness results for general rate-independent hysteresis problems*, Preprint no. 1078, WIAS, Berlin, 2005.

[56] A. Mielke, T. Roubíček, *Rate-independent damage processes in nonlinear elasticity*, Preprint no. 1020, WIAS, Berlin, 2005.

[57] A. Mielke, A. Timofte, *An energetic material model for time-dependent ferroelectric behavior: Existence and uniqueness*, Preprint no. 1014, WIAS, Berlin, 2005.

[58] P. Exner, T. Ichinose, H. Neidhardt, V. Zagrebnov, *Zeno product formula revisited*, Preprint no. 1053, WIAS, Berlin, 2005.

[59] H. Neidhardt, J. Rehberg, *Scattering matrix, phase shift, spectral shift and trace formula for one-dimensional Schrödinger-type operators*, Preprint no. 1045, WIAS, Berlin, 2005.

[60] ———, *Uniqueness for dissipative Schrödinger–Poisson systems*, Preprint no. 1044, WIAS, Berlin, 2005.

[61] J. Behrndt, H. Neidhardt, J. Rehberg, *Block operator matrices, optical potentials, trace class perturbations and scattering*, Preprint no. 1076, WIAS, Berlin, 2005.

[62] J. Polzehl, V. Spokoiny, *Structural adaptive smoothing by propagation-separation methods*, Preprint no. 1068, WIAS, Berlin, 2005.

[63] V.Z. Tronciu, H.-J. Wünsche, M. Radziunas, M. Wolfrum, *Semiconductor laser under resonant feedback from a Fabry–Perot: Stability of continuous wave operation*, Preprint no. 1051, WIAS, Berlin, 2005.

[64] A. Dalalyan, M. Reiss, *Asymptotic statistical equivalence for ergodic diffusions: The multidimensional case*, Preprint no. 1035, WIAS, Berlin, 2005.

[65] K.K. Sabelfeld, A. Levykin, T. Privalova, *A fast stratified sampling simulation of coagulation processes*, Preprint no. 1075, WIAS, Berlin, 2005.

[66] K.K. Sabelfeld, A. Levykin, I. Shalimova, *Random walk on fixed spheres method for electro- and elastostatics problems*, Preprint no. 1073, WIAS, Berlin, 2005.

[67] V. Kaganer, K. Ploog, K.K. Sabelfeld, *Dynamic coalescence kinetics of facetted 2D islands*, Preprint no. 1077, WIAS, Berlin, 2005.

[68] P. Kramer, O. Kurbanmuradov, K.K. Sabelfeld, *Extensions of multiscale Gaussian random field simulation algorithms*, Preprint no. 1040, WIAS, Berlin, 2005.

[69] O. Kurbanmuradov, K.K. Sabelfeld, *Exponential bounds for the probability deviations of sums of random fields*, Preprint no. 1036, WIAS, Berlin, 2005.

[70] ———, *Probability of error deviations for the dependent sampling Monte Carlo methods: Exponential bounds in the uniform norm*, Preprint no. 1015, WIAS, Berlin, 2005.

[71] ———, *Stochastic spectral and Fourier-wavelet methods for vector Gaussian random fields*, Preprint no. 1082, WIAS, Berlin, 2005.

[72] G. Hebermehl, J. Schefter, R. Schlundt, Th. Tischler, H. Zscheile, W. Heinrich, *Simulation of microwave and semiconductor laser structures including PML: Computation of the eigen mode problem, the boundary value problem, and the scattering matrix*, Preprint no. 1067, WIAS, Berlin, 2005.

[73] F. Lanzara, V. Maz'ya, G. Schmidt, *Approximate approximations from scattered data*, Preprint no. 1058, WIAS, Berlin, 2005.

[74] K. Tabelow, J. Polzehl, V. Spokoiny, *Analysing fMRI experiments with structural adaptive smoothing procedures*, Preprint no. 1079, WIAS, Berlin, 2005.

[75] A. Vladimirov, D. Skryabin, G. Kozyreff, P. Mandel, M. Tlidi, *Bragg localized structures in a passive cavity with transverse refractive index modulation*, Preprint no. 1049, WIAS, Berlin, 2005.

[76] M. Nizette, D.I. Rachinskii, A. Vladimirov, M. Wolfrum, *Pulse interaction via gain and loss dynamics in passive mode-locking*, Preprint no. 1060, WIAS, Berlin, 2005.

[77] S. Nagaev, V. Wachtel, *The critical Galton–Watson process without further power moments*, Preprint no. 1062, WIAS, Berlin, 2005.

[78] A. Münch, B. Wagner, Th.P. Witelski, *Lubrication models with small to large slip lengths*, Preprint no. 1069, WIAS, Berlin, 2005.

[79] M. Rauscher, A. Münch, B. Wagner, R. Blossey, *A thin-film equation for viscoelastic liquids of Jeffreys type*, Preprint no. 1012, WIAS, Berlin, 2005.

[80] J.R. King, A. Münch, B. Wagner, *Linear stability of a ridge*, Preprint no. 1070, WIAS, Berlin, 2005.

[81] A.L. Garcia, W. Wagner, *Generation of the Maxwellian inflow distribution*, Preprint no. 1013, WIAS, Berlin, 2005.

[82] S. Rjasanow, W. Wagner, *Stochastic weighted particle method – Theory and numerical examples*, Preprint no. 1021, WIAS, Berlin, 2005.

[83] R. Siegmund-Schultze, W. Wagner, *Induced gelation in a two-site spatial coagulation model*, Preprint no. 1037, WIAS, Berlin, 2005.

[84] K. Wilmanski, *Threshold to liquefaction in granular materials as a formation of strong wave discontinuity in poroelastic media*, Preprint no. 1003, WIAS, Berlin, 2005.

[85] S. Yanchuk, *Discretization of frequencies in delay coupled chaotic oscillators*, Preprint no. 1008, WIAS, Berlin, 2005.

A.7.2 WIAS Reports Series

[1] D. Belomestny, M. Reiss, *Optimal calibration of exponential Levy models*, WIAS Report no. 25, WIAS, Berlin, 2005.

A.7.3 Preprints/Reports in other Institutions

[1] M. Fischer, M. Reiss, *Discretisation of stochastic control problems for continuous time dynamics with delay*, Discussion paper no. 38, Humboldt-Universität zu Berlin, SFB 649, 2005.

[2] R. Henrion, *Structural properties of linear probabilistic constraints*, Preprint no. 13, Stochastic Programming E-Print Series (SPEPS), 2005.

[3] R. Henrion, W. Römisch, *Lipschitz and differentiability properties of quasi-concave and singular normal distribution functions*, Preprint no. 11, Stochastic Programming E-Print Series (SPEPS), 2005.

[4] D. Knees, *Griffith-formula and J-integral for a crack in a power-law hardening material*, Preprint no. 2005/12, Universität Stuttgart, SFB 404, 2005.

[5] D. Knees, A.-M. Sändig, *Regularity for nonlinear and linear PDEs in nonsmooth domains*, Preprint no. 2005/11, Universität Stuttgart, SFB 404, 2005.

[6] A. Zisowsky, A. Arnold, M. Ehrhardt, Th. Koprucki, *Discrete transparent boundary conditions for transient kp-Schrödinger equations with application to quantum heterostructures*, Preprint no. 166, DFG Priority Program "Analysis, Modeling and Simulation of Multiscale Problems", Stuttgart, 2005.

A.8 Talks, Posters, and Contributions to Exhibitions

A.8.1 Scientific Talks (Invited)

1. U. Bandelow, *Reduced amplitude noise in monolithic mode-locked semiconductor lasers*, Workshop on PHysics and Applications of SEmiconductor Lasers (PHASE 2005), March 29–30, Supélec — Ecole Supérieure d'Electricité, Metz, France, March 30.
2. ———, *Analyse dynamischer Effekte in Optoelektronik und Photonik*, Institutsseminar, Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin, December 9.
3. U. Bandelow, A. Demircan, *Impact of modulation instability on the supercontinuum generation*, 5th International Conference "Numerical Simulation of Optoelectronic Devices" (NUSOD'05), September 19–22, Humboldt-Universität zu Berlin, September 21.
4. M. Baro, *A quantum transmitting Schrödinger–Poisson system*, Physikalisches Kolloquium, Brandenburgische Technische Universität, Lehrstuhl Theoretische Physik, Cottbus, March 1.
5. D. Belomestny, *Efficient calibration of jump-diffusion LIBOR market model*, Université de Marne-la-Vallée, France, October 14.
6. Ch. Bender, *Strategieverbesserung für Amerikanische Optionen*, Martin-Luther-Universität Halle-Wittenberg, February 10.
7. ———, *A forward scheme for backward SDEs*, 4th Colloquium on BSDEs and their applications, May 30 – June 1, Shanghai, China, May 31.
8. ———, *Vorwärtssimulation von BSDEs*, Mathematisches Kolloquium, Technische Universität Braunschweig, Institut für Mathematische Stochastik, July 4.
9. M. Birkner, *Starke und schwache Unordnung für gerichtete Polymere in zufälliger Umgebung*, Oberseminar zur Mathematischen Stochastik, Johannes Gutenberg Universität Mainz, Institut für Angewandte Mathematik, January 18.
10. ———, *Wie schätzt man das Alter der mitochondrialen Eva? Wahrscheinlichkeitstheoretische Modelle in der Evolutionstheorie*, AG Bioinformatik, Johann Wolfgang Goethe-Universität Frankfurt, June 2.
11. ———, *Survival in the face of competition*, Meeting "Mathematical Population Genetics", August 21–27, Mathematisches Forschungsinstitut Oberwolfach, August 23.
12. ———, *A conditional large deviation principle and size biasing for linear systems*, BRG Workshop, October 12–14, EURANDOM, Eindhoven, The Netherlands, October 13.
13. J. Borchardt, *The block oriented process simulator BOP*, The Seventh Italian Conference on Chemical and Process Engineering (ICheaP-7), May 15–18, Giardini di Naxos, Italy, May 18.
14. A. Bovier, *Nucléation dans la dynamique de Kawasaki à basse température*, Seminaire de Probabilité, Université Paris VI, France, March 1.
15. ———, *Valeurs propres principales dans des modèles de selection-mutation*, Université Paris X, France, March 24.
16. ———, *On the Mertens universality conjecture*, Workshop "Spin Glasses and Scaling Limits in Physics", May 1–4, Universität Bielefeld, Zentrum für interdisziplinäre Forschung (ZiF), May 4.
17. ———, *Energy level statistics in disordered systems: The local REM conjecture and beyond*, Workshop "Applications of Random Matrices in Economics and other Complex Systems", May 25–28, Jagiellonian University, Cracow, Poland, May 27.
18. ———, *The local REM conjecture and beyond*, Workshop "Mathematical Physics of Spin Glasses", June 27 – July 2, Istituto Nazionale di Alta Matematica (INDAM), Cortona, Italy, July 2.

19. ———, *Ageing and spectral properties of generators*, Workshop "Stochastic Partial Differential Equations and Random Media: From Theory to Applications II", September 2–16, Universität Bielefeld, Zentrum für interdisziplinäre Forschung (ZiF), September 15.
20. ———, *Towards a spectral approach to ageing*, Workshop "Interacting Stochastic Systems", September 20–22, EURANDOM, Eindhoven, The Netherlands, September 21.
21. ———, *Universality in the local energy statistics in disordered spin systems*, Technion—Israel Institute of Technolgy, Willam Davidson Faculty of Industrial Engineering and Management, Haifa, December 28.
22. J. Cerny, *Aging in trap models, convergence to the arc-sine law*, Workshop "Spin Glasses and Scaling Limits in Physics", May 2–4, Universität Bielefeld, Zentrum für interdisziplinäre Forschung (ZiF), May 2.
23. ———, *Aging in trap models, convergence to the arc-sine law*, Workshop "Metastability, ageing, and anomalous diffusion: Stochastic and nonlinear effects in long term dynamics", Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, May 20.
24. ———, *Ageing in trap models, singular diffusions and convergence to the arc-sine law*, University of Oxford, The Mathematical Institute, UK, May 23.
25. ———, *Stock price evolution from microscopic market modelling*, Rhein-Main-Kolloquium Stochastik, Johann Wolfgang Goethe-Universität Frankfurt, June 22.
26. ———, *Aging and the arc-sine law*, Summer School "Mathematical Statistical Physics", July 4–29, "École d'Été de Physique Théorique", Les Houches, France, July 29.
27. N. Champagnat, *A microscopic interpretation for a Markov jump process of evolution in adaptive dynamics*, Workshop "Spin Glasses and Scaling Limits in Physics", August 17–19, Universität Bielefeld, Zentrum für interdisziplinäre Forschung (ZiF), August 18.
28. ———, *A microscopic interpretation for a Markov jump model of evolution in adaptive dynamics*, Meeting "Mathematical Population Genetics", August 21–27, Mathematisches Forschungsinstitut Oberwolfach, August 25.
29. ———, *From microscopic to macroscopic ecological stochastic models of evolution*, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, October 27.
30. Y. Chen, *GHICA — Risk analysis with GH distributions and independent components*, First Closed Meeting of SFB 649, June 23–25, Motzen, June 23.
31. A. Demircan, U. Bandelow, *Impact of modulation instability on supercontinuum generation*, Annual Meeting 2005 of the Optical Society of America (OSA) "Frontiers in Optics", October 17–21, Tuscon, USA, October 19.
32. W. Dreyer, *On dynamics of phase transitions in crystalline solids*, Institut für Kristallzüchtung, Berlin, January 14.
33. ———, *Thermodynamics of the Becker/Döring system*, International Conference "Free Boundary Problems: Theory and Applications", June 7–12, Coimbra, Portugal, June 8.
34. ———, *Thermodynamic modeling and analysis of phase transitions*, Philips, Eindhoven, The Netherlands, August 16.
35. ———, *Zur Evolution flüssiger Ausscheidungen in kristallinen Festkörpern*, 18. Workshop "Composite Forschung in der Mechanik", December 6–7, Universität Paderborn, December 6.
36. J. Elschner, *Inverse Probleme für optische Gitter*, Physikalisch-Technische Bundesanstalt, Berlin, April 13.
37. ———, *Inverse problems for diffraction gratings*, Inverse Scattering Workshop, University of North Carolina, Charlotte, USA, June 3.
38. ———, *Inverse problems for diffraction gratings*, University of Delaware, Department of Mathematics, Newark, USA, June 9.

39. K. Eppler, *Shape optimization for elliptic free boundary problems*, Utrecht University, Department of Mathematics, The Netherlands, March 1.

40. ———, *Exterior electromagnetic shaping: AD-based computation of shape derivatives*, GAMM Annual Meeting 2005, March 29 – April 1, Luxemburg, March 29.

41. ———, *Shape optimization algorithms using wavelet-based BEM*, Third M.I.T. Conference on Computational Fluid and Solid Mechanics, June 14–17, Cambridge, USA, June 15.

42. ———, *Fast BEM methods for the efficient treatment of elliptic shape optimization problems*, Third M.I.T. Conference on Computational Fluid and Solid Mechanics, June 14–17, Cambridge, USA, June 16.

43. ———, *Exterior electromagnetic shaping: Analytic and AD-based computation of shape derivatives*, 22nd IFIP TC 7 Conference on System Modeling and Optimization, July 18–22, Turin, Italy, July 21.

44. ———, *Treating the EIT problem by higher order shape calculus — the (n+1)st explanation for exponential ill-posedness*, Chemnitzer Minisymposium zu Inversen Problemen, September 15.

45. M.H. Farshbaf Shaker, *On a nonlocal Cahn–Hillard equation*, Max-Planck-Institut für Mathematik in den Naturwissenschaften, AG Mikrostrukturen, Leipzig, November 29.

46. M. Fischer, *Numerical approximate for stochastic control problems with time delay*, Università di Roma "La Sapienza", Dipartimento di Matematica, Italy, September 28.

47. J. Fuhrmann, *Numerical simulation of Direct Methanol Fuel Cells*, BIRS Workshop "Computational Fuel Cell Dynamics III", March 19–24, Banff International Research Station, Canada, March 24.

48. ———, *Finite volume schemes for nonlinear convection-diffusion problems based on the solution of local Dirichlet problems*, EQUADIFF 11 International conference on differential equations, July 25–29, Comenius University, Bratislava, Slovakia, July 28.

49. K. Gärtner, *3D simulations of DEPFET-based sensors: Algorithms and results*, 5th International Conference "Numerical Simulation of Optoelectronic Devices" (NUSOD 05), September 19–22, Humboldt-Universität zu Berlin, September 21.

50. J. Geiser, *Modified discretization methods with embedded analytical solutions based on finite volume and discontinuous Galerkin methods and some applications in porous media*, Third M.I.T. Conference on Computational Fluid and Solid Mechanics, June 14–17, Cambridge, USA, June 15.

51. ———, *Discretization methods for hyperbolic and parabolic equations based on finite volume and related methods and their applications in fluid- and gas-mechanics*, Eighth U.S. National Congress on Computational Mechanics, Session: Complex Models in Solid and Fluid Mechanics, July 24–28, Austin, USA, July 26.

52. ———, *Discretization-optimization methods for nonlinear parabolic optimal control problems with state constraint*, Workshop "Analysis and Optimization", National Technical University of Athens, Department of Applied Mathematics and Physics, Greece, September 20.

53. B. Gentz, *Residence-time distributions as a measure for stochastic resonance*, Workshop "Stochastic Climate Models", May 30 – June 1, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, June 1.

54. ———, *Dansgaard–Oeschger events, residence-times, and stochastic resonance*, ZiF Conference "Stochastic Partial Differential Equations and Climatology", June 8–10, Universität Bielefeld, Zentrum für interdisziplinäre Forschung (ZiF), June 9.

55. ———, *The effect of noise on slow–fast systems*, Summer School "Mathematical Statistical Physics", July 4–29, "École d'Été de Physique Théorique", Les Houches, France, July 11.

56. J. Giannoulis, *Pulse propagation in discrete lattices*, Workshop on Dynamical Problems in Mathematical Materials Science, July 18–22, International Centre for Mathematical Sciences of Edinburgh University and Heriot–Watt University, Edinburgh, UK, July 18.

57. A. GLITZKY, *An application of the Implicit Function Theorem to stationary energy models for semiconductor devices*, International Workshop "Regularity for nonlinear and linear PDEs in nonsmooth domains", September 4–7, Universität Stuttgart, Hirschegg, Austria, September 5.
58. J.A. GRIEPENTROG, *On a nonlocal image segmentation and reconstruction algorithm*, ALGORITMY 2005 – 17th Conference on Scientific Computing, March 13–18, Vysoke Tatry/Podbanske, Slovakia, March 14.
59. R. HENRION, *Some contributions to the theory and numerics of chance-constrained programming*, Charles University, Department of Probability and Mathematical Statistics, Prague, Czech Republic, March 3.
60. ———, *Calculating values and gradients of polyhedral chance constraints*, MATHEON MF 1 Workshop "Optimization Software", Konrad-Zuse-Zentrum für Informationstechnik Berlin, June 1.
61. ———, *Calmness of chance constraints and Lipschitz properties of the value-at-risk*, 22nd IFIP TC 7 Conference on System Modeling and Optimization, July 18–22, Turin, Italy, July 21.
62. ———, *Stability of solutions in programs with probabilistic constraints*, 10-th Workshop on Well-posedness of Optimization Problems and Related Topics, September 5–9, Borovets, Bulgaria, September 9.
63. ———, *Optimization problems with linear chance constraints — structure, numerics and applications*, 75th Meeting of Gesellschaft für Operations Research (GOR) Workgroup "Praxis der Mathematischen Optimierung": Optimization Under Uncertainty, October 20–21, Bad Honnef, October 21.
64. ———, *Properties of linear probabilistic constraints*, INFORMS Annual Meeting, November 13–16, San Francisco, USA, November 14.
65. ———, *Stochastische Optimierungsprobleme mit "chance constraints"*, Universität Stuttgart, Institut für Stochastik und Anwendungen, December 15.
66. R. HENRION, T. SZÁNTAI, *Properties and calculation of singular normal distributions*, Dagstuhl Seminar on "Algorithms for Optimization with Incomplete Information", Schloss Dagstuhl, January 17.
67. D. HÖMBERG, *Optimal control of solid-solid phase transitions including mechanical effects*, Workshop "Optimal Control of Coupled Systems of PDE", April 17–23, Mathematisches Forschungsinstitut Oberwolfach, April 22.
68. ———, *A thermomechanical phase transition model for the surface hardening of steel*, International Conference "Free Boundary Problems: Theory and Applications", June 7–12, Coimbra, Portugal, June 11.
69. ———, *Die Laserhärtung von Stahl — Modellierung, Analysis und optimale Steuerung*, Universität Bayreuth, Mathematisches Institut, June 30.
70. ———, *On a thermomechanical model of surface heat treatments*, EQUADIFF 11 International conference on differential equations, July 25–29, Comenius University, Bratislava, Slovakia, July 28.
71. ———, *Control of laser material treatments*, SIAM Conference on Mathematics for Industry, October 24–26, Detroit Marriott Renaissance Center, USA, October 25.
72. ———, *Laser material treatments — modeling, simulation, and optimal control*, Michigan State University, Department of Mathematics, East Lansing, USA, October 27.
73. ———, *Von der Stahlhärtung bis zur Krebstherapie — Simulations- und Optimierungsaufgaben in Lehre und Forschung*, FEMLAB Konferenz 2005, November 3–4, Frankfurt am Main, November 3.
74. ———, *Modelling, simulation and control of laser material treatments*, Scuola Normale Superiore, Pisa, Italy, November 22.
75. H.-CHR. KAISER, *Quasi-3D simulation of multi-excitons by means of density functional theory*, Oberseminar "Numerik/Wissenschaftliches Rechnen", Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, January 11.
76. ———, *Modeling and quasi-3D simulation of indium grains in (In,Ga)N/GaN quantum wells by means of density functional theory*, Physikalisches Kolloquium, Brandenburgische Technische Universität, Lehrstuhl Theoretische Physik, Cottbus, February 15.

77. ———, *An open quantum system driven by an external flow*, Workshop "Nonlinear spectral problems in solid state physics", April 4–8, Institut Henri Poincaré, Paris, France, April 7.
78. ———, *Spectral resolution of a velocity field on the boundary of a Lipschitz domain*, 2nd Joint Meeting of AMS, DMV, ÖMG, June 16–19, Johannes Gutenberg-Universität, Mainz, June 16.
79. ———, *About quantum transmission on an up to three dimensional spatial domain*, University of Texas at Dallas, USA, October 28.
80. ———, *On quantum transmission*, Mathematical Physics Seminar, November 9–11, University of Texas at Austin, USA, November 9.
81. O. Klein, *Outward pointing properties for Preisach operators*, 5th International Symposium on Hysteresis and Micromagnetic Modeling (HMM 2005), May 30 – June 1, Budapest, Hungary, May 30.
82. D. Knees, *Global regularity of the elastic fields of a power-law model on nonsmooth domains*, Offenes Seminar "Partielle Differentialgleichungen und Anwendungen", Technische Universität Darmstadt, Fachbereich Mathematik, November 8.
83. P. Krejčí, *Well-posedness of macroscopic models of fatigue driven by changes of microstructure*, 4th GAMM Seminar on Microstructures, January 14–16, Bedlewo, Poland, January 14.
84. ———, *Asymptotic properties of a phase transition model*, Seminar of Partial Differential Equations, Czech Academy of Sciences, Mathematical Institute, Prague, April 5.
85. ———, *Asymptotic hysteresis patterns in a phase separation problem*, International Conference "Free Boundary Problems: Theory and Applications", June 7–12, Coimbra, Portugal, June 11.
86. ———, *Long time behaviour of a singular phase transition model*, Meeting "Evolution Equations: Inverse and Direct Problems", June 20–24, Cortona, Italy, June 21.
87. ———, *Nonresonance and energy decay of oscillations in hysteretic media*, EQUADIFF 11 International conference on differential equations, July 25–29, Comenius University, Bratislava, Slovakia, July 25.
88. ———, *Hystereze v rovnicích s malým parametrem (in Czech)*, Seminar "Determinismus a chaos", September 5–7, Herbertov, Czech Republic, September 5.
89. P. Mathé, *Uniform function estimation under general smoothness*, Georg-August-Universität Göttingen, Mathematische Fakultät, April 20.
90. ———, *Interpolation in variable Hilbert scales with application to inverse problems*, Technische Universität Chemnitz, September 15.
91. ———, *Variable Hilbert scales. Interpolation and approximation*, Beijing Normal University, China, October 12.
92. ———, *Computing functionals of large scale matrices*, Beijing Normal University, China, October 14.
93. A. Mielke, *Macroscopic equations for microscopic dynamics in periodic crystals*, IMA Workshop "Atomic Motion to Macroscopic Models: The Problem of Disparate Temporal and Spatial Scales", April 11–15, Institute for Mathematics and Its Applications (IMA), Minneapolis, USA, April 13.
94. ———, *Ratenunabhängige Modelle für die Elastoplastizität bei finiten Deformationen*, Seminar für Rechnergestützte Mechanik, colloquium in the framework of SFB 551, Universität Karlsruhe, Institut für Technische Mechanik, June 23.
95. ———, *Space-time chaos in reaction-diffusion systems*, Mini-symposium "Nonlinear Analysis and Applications", Universität Augsburg, Institut für Mathematik, June 24.
96. ———, *Macroscopic equations for microscopic dynamics in periodic crystals*, Workshop on Dynamical Problems in Mathematical Materials Science, July 18–23, International Centre for Mathematical Sciences of Edinburgh University and Heriot-Watt University, Edinburgh, UK, July 18.
97. ———, *Energetic formulation of hysteresis problems, existence and uniqueness*, EQUADIFF 11 International conference on differential equations, July 25–29, Comenius University, Bratislava, Slovakia, July 25.

98. ———, *Dynamics of modulated pulses in discrete lattices via the nonlinear Schrödinger equation*, 4th International Workshop "Successes and Failures of Continuous Models for Discrete Systems", September 5–9, University of Bristol, UK, September 9.

99. ———, *Evolution of microstructure in shape-memory alloys: Analysis and numerics*, 1st International Conference "Multi-scale problems: Modelling, analysis and applications", September 12–14, University of Bath, Bath Institute for Complex Systems (BICS), UK, September 12.

100. ———, *Mathematische Methoden in den Materialwissenschaften*, 6 talks, Vacation Academy 2005 of Technische Universität München, Friedrich-Alexander-Universität Erlangen–Nürnberg, and Universität Stuttgart, Sarntal, Italy, September 25–29.

101. ———, *Noncompact Lie groups, polyconvexity and finite-strain elastoplasticity*, International Symposium on Mathematical Sciences in honor of Eberhard Zeidler on the occasion of his 65th birthday, October 6–8, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, October 8.

102. ———, *Some existence results for finite-strain plasticity*, Mini-Workshop "Analysis and Computation of Microstructures in Finite Plasticity", November 13–19, Mathematisches Forschungsinstitut Oberwolfach, November 15.

103. ———, *Propagation of waves in discrete periodic lattices*, Séance du Groupe de Travail "Mécanique des Fluides", Université Paul Sabatier, Laboratoire MIP, Toulouse, France, December 15.

104. H.-J. Mucha, *Informative Dendrogramme*, 4th SPSS Academic Convention, June 8–9, Potsdam, June 9.

105. H. Neidhardt, *Zeno product formula and continual observations in quantum mechanics*, Workshop on Operator Semigroups, Evolution Equations, and Spectral Theory in Mathematical Physics, October 3–7, Centre International de Rencontres Mathématiques, Marseille, France, October 5.

106. ———, *A quantum transmitting Schrödinger–Poisson system*, Workshop "Quantum Transport and Exitations from Macro to Nanoscale: Theory and Applications", November 10–13, Aalborg University, Denmark, November 11.

107. ———, *Hybrid models for semiconductors*, Physikalisches Kolloquium, Brandenburgische Technische Universität Cottbus, Lehrstuhl für Theoretische Physik, November 29.

108. J. Polzehl, *Propagation-separation at work: Main ideas and applications*, National University of Singapore, Department of Probability Theory and Statistics, March 24.

109. ———, *Adaptive smoothing by propagation-separation*, Australian National University, Center of Mathematics and its Applications, Canberra, March 31.

110. ———, *Image reconstruction and edge enhancement by structural adaptive smoothing*, 55th Session of the International Statistical Institute (ISI), April 5–12, Sydney, Australia, April 8.

111. ———, *Spatially adaptive smoothing: A propagation-separation approach for imaging problems*, Joint Statistical Meetings, August 7–11, Minneapolis, USA, August 11.

112. ———, *Structural adaptive smoothing by propagation-separation methods*, Ludwig-Maximilians-Universität München, SFB 386, December 7.

113. D. Rachinskii, *Bifurcations in systems with complex nonlinearities*, Technische Universität München, February 21.

114. J. Rademacher, *Bifurcations from heteroclinic cycles with a periodic orbit*, Weekly Informal Seminar, University of Surrey, Department of Mathematics, Guildford, UK, October 25.

115. ———, *Essential and absolute spectra, and their computation by continuation*, Program: Pattern Formation in Large Domains, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, October 28.

116. ———, *Pulse motion on a uniformly growing interval in the semi-strong limit of the Schnakenberg model*, Program: "Pattern Formation in Large Domains", Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, November 1.

117. ———, *Computing absolute and essential spectra using continuation*, Nonlinear Analysis Seminar, University of Bristol, Engineering Mathematics Department, Great Britain, December 14.

118. M. RADZIUNAS, *Numerical bifurcation analysis of the traveling wave model of multisection semiconductor lasers*, Workshop "Qualitative Numerical Analysis of High-dimensional Nonlinear Systems", March 21–24, University of Bristol, UK, March 23.

119. A. RATHSFELD, *Integralgleichungsmethode für optische Gitter — Weiterentwicklung der IESMP*, Kick-off Meeting of BMBF Project "NAOMI", Carl Zeiss AG, Jena, May 31.

120. ———, *Optimization of diffraction gratings with* DiPoG, MATHEON MF 1 Workshop "Optimization Software", Konrad-Zuse-Zentrum für Informationstechnik Berlin, June 1.

121. ———, *Finite elements for the rigorous simulation of time-harmonic waves*, 3rd IISB Lithography Simulation Workshop, September 16–18, Pommersfelden, September 16.

122. ———, *Optimierung von optischen Gittern mit* DiPoG-2.1, 2nd Meeting "Inverses Problem in der Scatterometrie", Physikalisch-Technische Bundesanstalt, Braunschweig, October 18.

123. J. REHBERG, *Some analytical ideas concerning the quantum-drift-diffusion systems*, Workshop "Problèmes spectraux non-linéaires et modèles de champs moyens", April 4–8, Institut Henri Poincaré, Paris, France, April 5.

124. ———, *Elliptische und parabolische Probleme aus Anwendungen*, Kolloquium im Fachbereich Mathematik, Universität Darmstadt, May 18.

125. ———, *Existence, uniqueness and regularity for quasilinear parabolic systems*, Conference "Nonlinear Parabolic Problems", October 17–21, Finnish Mathematical Society (FMS), University of Helsinki, and Helsinki University of Technology, Finland, October 20.

126. ———, *Analysis of macroscopic and quantum mechanical semiconductor models*, International Visitor Program "Nonlinear Parabolic Problems", August 8 – November 18, Finnish Mathematical Society (FMS), University of Helsinki, and Helsinki University of Technology, Finland, November 1.

127. ———, *Regularität für elliptische Probleme mit unglatten Daten*, Oberseminar Prof. Escher/Prof. Schrohe, Technische Universität Hannover, December 13.

128. K.K. SABELFELD, *Random walk methods for solving stochastic elasticity problems*, International Conference on Selected Problems of Modern Mathematics, April 4–8, Kaliningrad, Russia, April 4.

129. ———, *A method of random walks on fixed spheres for solving Neumann and mixed Neumann–Dirichlet boundary value problems*, Vth IMACS Seminar on Monte Carlo Methods (MCM 2005), May 16–20, Tallahassee, USA, May 17.

130. ———, *A fast direct Monte Carlo simulation of coagulation processes*, Vth IMACS Seminar on Monte Carlo Methods (MCM 2005), May 16–20, Tallahassee, USA, May 18.

131. ———, *Stochastic flow simulation in porous media*, Vth IMACS Seminar on Monte Carlo Methods (MCM 2005), May 16–20, Tallahassee, USA, May 18.

132. ———, *Extensions of multiscale Gaussian random field simulation algorithms*, Vth IMACS Seminar on Monte Carlo Methods (MCM 2005), May 16–20, Tallahassee, USA, May 20.

133. ———, *New stochastic simulation methods for solving coagulation problems with applications to polymer modelling*, University of Cambridge, Department of Chemical Engineering, UK, June 24.

134. G. SCHMIDT, *Simulation und Optimierung periodischer diffraktiver Strukturen mit DiPoG*, Physikalisch-Technische Bundesanstalt, Berlin, April 13.

135. ———, *Scattered data approximation*, Università degli Studi di Roma "La Sapienza", Dipartimento di Metodi e Modelli Matematici, Italy, July 22.

136. J.G.M. SCHOENMAKERS, *Iterative construction of the optimal Bermudan stopping time*, Frankfurt MathFinance Workshop "Derivatives and risk management in theory and practice", April 14–15, HfB — Business School of Finance and Management, Frankfurt am Main, April 14.

137. ———, *Robust Libor modelling and pricing of derivative products*, Delft University of Technology, The Netherlands, June 9.

138. H. Si, *TetGen, a 3D quality mesh generator, algorithms and examples*, Technische Universität Darmstadt, Fachbereich Mathematik, July 5.

139. V. Spokoiny, *GARCH versus local constant volatility modeling. Comparison of the predictive power*, STATDEP 2005, Statistics for Dependent Data, January 26–29, Centre de Recherche en Economie et Statistiques, Laboratoire de Statistiques, Paris, France, January 29.

140. ———, *Varying coefficient GARCH versus local constant volatility modeling*, Hejnice Compact Seminar (SFB 649), February 10–13, International Centre for Spiritual Rehabilitation, Hejnice, Czech Republic, February 12.

141. ———, *Varying coefficient GARCH versus local constant modelling*, Workshop on Semi-parametric Methods for Survival and Longitudinal Data, March 17–20, National University of Singapore, March 18.

142. ———, *Spatially adaptive local likelihood modelling via stagewise aggregation*, Universität Lübeck, Institut für Neuro- und Bioinformatik, May 20.

143. ———, *Local parametric approach in nonparametric estimation*, 4 talks, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, June 10–21.

144. ———, *Local parametric approach in nonparametric estimation*, Workshop "Statistische und Probabilistische Methoden der Modellwahl", October 16–22, Mathematisches Forschungsinstitut Oberwolfach, October 19.

145. ———, *Moderne Methoden der Bildverarbeitung*, Bundesanstalt für Materialforschung und -prüfung, Berlin, October 28.

146. J. Sprekels, *Nonlocal phase-field models for nonisothermal phase transitions*, International Conference "Free Boundary Problems: Theory and Applications", June 7–12, Coimbra, Portugal, June 8.

147. ———, *Modeling and control of curved mechanical structures*, Meeting "Evolution Equations: Inverse and Direct Problems", June 20–24, Cortona, Italy, June 21.

148. K. Tabelow, *Adaptive weights smoothing in the analysis of fMRI data*, Ludwig-Maximilians-Universität München, SFB 386, December 8.

149. A. Vladimirov, *Interaction of dissipative solitons in laser systems*, Ben Gurion University of the Negev, Department of Mathematics, Beer Sheva, Israel, November 17.

150. A. Vladimirov, G. Kozyreff, P. Mandel, M. Tlidi, *Localized structures in a passive cavity with refractive index modulation*, International Quantum Electronics Conference, June 12–17, München, June 15.

151. A. Vladimirov, D. Turaev, D. Rachinskii, *Delay differential models of mode-locking in semiconductor lasers*, International Conference on Coherent and Nonlinear Optics, May 11–16, St. Petersburg, Russia, May 14.

152. B. Wagner, *The role of slippage for dewetting fronts in thin polymer films*, International Conference "Free Boundary Problems: Theory and Applications", June 7–12, Coimbra, Portugal, June 10.

153. ———, *The role of slippage in dewetting fronts in thin polymer films*, 2005 SIAM Annual Meeting, July 11–15, New Orleans, USA, July 14.

154. ———, *Lubrication models for small to large slip lengths*, Summer Workshop of the DFG Priority Program SPP 1164: "Nano- and Microfluidics: Bridging the Gap between Molecular Motion and Continuum Flow", August 17–19, Bad Honnef, August 17.

155. W. Wagner, *Stochastic models for coagulation-fragmentation processes*, Workshop on Coagulation-Fragmentation Processes: Theory and Application, July 4–8, University of Edinburgh, UK, July 5.

156. ———, *Stochastic models and Monte Carlo algorithms for nonlinear kinetic equations*, September 10–29, Los Alamos National Laboratories, USA, September 12.

157. ———, *Generation of the Maxwellian inflow distribution*, Conference "Direct Simulation Monte Carlo: Theory, Methods and Applications", September 26–29, Santa Fe, USA, September 26.

158. W. Weiss, *Extended thermodynamics with consistent order*, XIII International Conference on Waves and Stability in Continuous Media (WASCOM), June 19–25, Acireale, Italy, June 24.

159. ———, *Bizarres, Erheiterndes und ernste Begebenheiten zur Entdeckung der beiden Hauptsätze der Thermodynamik*, Deutsche Gesellschaft für Zerstörungsfreie Prüfung e.V., Bundesanstalt für Materialforschung und -prüfung, Berlin, December 6.

160. M. Wolfrum, *Systems of delay differential equations with large delay*, Otto-von-Guericke-Universität Magdeburg, Institut für Analysis und Numerik, June 14.

161. ———, *Synchronous and asynchronous instabilities of two lasers with a long delayed coupling*, EUROMECH Nonlinear Dynamics Conference (ENOC 2005), August 7–12, Eindhoven, The Netherlands, August 8.

162. S. Yanchuk, *Appearance of patterns in delay coupled laser arrays*, Universität Potsdam, January 31.

163. ———, *Bifurcations in systems with large delay*, SFB 555 Symposium, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, May 27.

164. ———, *Normal forms for systems with large delay*, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, October 10.

A.8.2 Talks for a More General Public

1. M. Birkner, *Wie schätzt man das Alter der mitochondrialen Eva? Wahrscheinlichkeitstheoretische Modelle in der Evolutionstheorie*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2005, WIAS, June 11.

2. J. Fuhrmann, *Brennstoffzellen im Computer*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2005, WIAS, June 11.

3. K. Gärtner, *Halbleitersensoren für Astronomie und Hochenergiephysik: Rechnen und Nachdenken, so unterscheidet man auch noch die Farbe des nachzuweisenden Lichts*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2005, WIAS, June 11.

4. B. Gentz, *Die Mathematik der Eiszeiten*, Marie-Curie-Gymnasium, Ludwigsfelde, November 10.

5. D. Hömberg, *Was erforscht eigentlich ein angewandter Mathematiker?*, WIAS, April 29.

6. G. Reinhardt, *Grundlagen zur (computergestützten) Bearbeitung von digitalen Bildern*, 10. Berliner Tag der Mathematik (10th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, June 4.

7. J. Sprekels, *Wie kann ich meinen Arbeitsaufwand optimieren, um ein Examen zu bestehen?*, 10. Berliner Tag der Mathematik (10th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, June 4.

8. H. Stephan, *Der kürzeste Weg in Geometrie und Analysis*, 10. Berliner Tag der Mathematik (10th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, June 4.

9. W. Weiss, *Außen hart und innen weich*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2005, WIAS, June 11.

A.8.3 Posters

1. U. Bandelow, A. Demircan, *Impact of the modulation instability on supercontinuum generation*, Conference on Lasers and Electro-Optics/Quantum Electronics & Lasers Science Conference CLEO/QELS 2005, München, June 12–17.

2. G. Enchéry, J. Fuhrmann, U. Bayer, F. Magri, H.-J. Diersch, V. Clausnitzer, A. Pekdeger, M. Tesmer, H.-J. Voigt, C. Jahnke, P. Möller, *Comparison of numerical methods in solving density driven fluid flow*, DFG Priority Program SPP 1135, Paderborn, November 30 – December 2.
3. M.H. Farshbaf Shaker, *On a nonlocal Cahn–Hillard–Gurtin equation*, International Conference "Free Boundary Problems: Theory and Applications", Coimbra, Portugal, June 7–12.
4. K. Gärtner, H. Gajewski, *A nonlocal phase segregation model, dissipative discretization and pattern formation*, XXV European Dynamics Day 2005, Technische Universität Berlin, July 25–28.
5. K. Gärtner, R. Richter, *Application of an experimental device simulation code to 3D DEPFET based sensor designs*, 10th European Symposium on Semiconductor Detectors, Wildbad Kreuth, June 12–16.
6. J. Giannoulis, *Pulse propagation in oscillator chains*, 1st Conference "Multi-scale Problems: Modelling, Analysis and Applications", Bath, UK, September 12–14.
7. ———, *Pulse propagation in oscillator chains*, 4th International Workshop "Successes and Failures of Continuous Models for Discrete Systems", Bristol, UK, September 5–8.
8. A. Mielke, J. Giannoulis, *Macroscopic dynamics in discrete lattices*, IMA Workshop "Atomic Motion to Macroscopic Models: The Problem of Disparate Temporal and Spatial Scales in Matter", Minneapolis, USA, April 11–15.
9. M. Radziunas, H.-J. Wünsche, V. Tronciu, *Stability of continuous wave states in semiconductor laser with external resonator*, Workshop on PHysics and Applications of SEmiconductor Lasers (PHASE 2005), Supélec — Ecole Supérieure d'Electricité, Metz, France, March 29–30.
10. M. Radziunas, U. Bandelow, M. Wolfrum, A. Glitzky, R. Hünlich, U. Troppenz, J. Kreissl, *Design of multisection semiconductor laser for 40 Gb/s direct modulation*, 31st European Conference on Optical Communication ECOC 2005, Glasgow, UK, September 25–29.
11. A. Rathsfeld, *Local optimization of polygonal gratings for classical and conical diffraction*, Conference "Diffractive Optics 2005", Warsaw, Poland, September 3–7.
12. K. Tabelow, J. Polzehl, *Structure adaptive smoothing procedures in medical imaging*, 19. Treffpunkt Medizintechnik "Imaging und optische Technologien für die Medizin", Berlin, June 1.
13. B. Tollkühn, M. Uhle, J. Fuhrmann, K. Gärtner, A. Heubner, A. Erdmann, *Benchmark of a lithography simulation tool for next generation applications*, International Conference on Micro- and Nano-Engineering (MNE-2005), Vienna, Austria, September 19–22.
14. D. Turaev, S. Zelik, A. Vladimirov, *Chaotic bound state of localized structures in the complex Ginzburg–Landau equation*, Conference Digest "Nonlinear Guided Waves and their Applications", Dresden, September 6–9.
15. M. Nizette, A. Vladimirov, M. Wolfrum, D. Rachinskii, *Delay differential equations for passive mode-locking*, International Quantum Electronics Conference, München, June 12–17.
16. S. Yanchuk, *Discretization of frequencies in coupled chaotic oscillators*, XXV Dynamics Days Europe 2005, Technische Universität Berlin, July 25–28.

A.8.4 Contributions to Exhibitions

1. U. Bandelow, *Presenting WIAS*, LASER 2005. World of Photonics, June 13–16, München, June 15.

A.9 Visits to other Institutions[4]

1. Ch. Bender, Universtät Konstanz, Fachbereich Mathematik und Statistik, January 20 – February 6.
2. ———, Helsinki University of Technology, Institute of Mathematics, Finland, May 10–25.
3. ———, Technische Universität Braunschweig, Institut für Mathematische Stochastik, November 1, 2005 – February 28, 2006.
4. M. Birkner, Johannes Gutenberg-Universität Mainz, Institut für Mathematik, January 18–21.
5. ———, University of Oxford, Department of Mathematics, UK, February 27 – March 4.
6. A. Bovier, European Science Foundation, Programme RDSES, Université Paris IV, Laboratoire de Probabilités, Paris, France, February 21 – March 6.
7. ———, Universität Bielefeld, Zentrum für interdisziplinäre Forschung (ZIF), September 1–16.
8. ———, Université Paris IV, Laboratoire de Probabilités, France, November 7–13.
9. ———, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, December 17, 2005 – January 8, 2006.
10. J. Cerny, University of Oxford, Department of Mathematics, UK, May 22 – June 24.
11. J. Elschner, University of Tokyo, Department of Mathematical Sciences, Japan, January 30 – February 26.
12. ———, University of Delaware, Department of Mathematical Sciences, Newark, USA, June 3–10.
13. K. Eppler, Utrecht University, Department of Mathematics, The Netherlands, February 28 – March 4.
14. M. Fischer, Ruprecht-Karls-Universität Heidelberg, Institut für Angewandte Mathematik, November 28 – December 2.
15. ———, Universitá di Roma I “La Sapienza”, Dipartimento di Matematica, Italy, December 15–23.
16. K. Fleischmann, University of Bath, Department of Mathematical Sciences, UK, June 20–25.
17. B. Gentz, CNRS-Centre de Physique Théorique, Marseille, France, November 24 – December 5.
18. R. Henrion, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, February 28 – March 4.
19. D. Knees, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, August 22 – September 9.
20. P. Mathé, Technische Universität Chemnitz, Fakultät für Mathematik, September 12–16.
21. ———, Beijing Normal University, School of Mathematical Sciences, China, October 8–19.
22. J. Polzehl, National University of Singapore, Department of Probability Theory and Statistics, March 23–29.
23. ———, Australian National University, Center of Mathematics and its Applications, Canberra, March 30 – April 4.
24. ———, University of Minnesota, School of Statistics, Minneapolis, USA, July 18 – August 14.
25. J. Rehberg, Helsinki University of Technology, Institute of Mathematics, Finland, October 19 – November 4.
26. M. Reiss, Université de Marne-la-Vallée, Laboratoire d’Analyse et de Mathématiques Appliquées, France, March 4–9.
27. K.K. Sabelfeld, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, December 7, 2004 – January 14, 2005.
28. ———, Florida State University, Department of Computer Sciences, Tallahassee, USA, May 16–22.

[4] Only stays of more than three days are listed.

29. ———, University of Cambridge, Department of Chemical Engineering, UK, June 22–26.
30. ———, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, July 25 – September 4.
31. ———, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, December 19, 2005 – January 27, 2006.
32. G. SCHMIDT, Università degli Studi di Roma "La Sapienza", Dipartimento di Metodi e Modelli Matematici, Italy, July 19 – August 23.
33. V. SPOKOINY, National University of Singapore, Department of Mathematics, February 21 – March 20.
34. ———, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, June 6–23.
35. A. VLADIMIROV, Free University of Brussels, Belgium, February 28 – March 12.
36. ———, Ben Gurion University of the Negev, Department of Mathematics, Beer Sheva, Israel, November 10–24.
37. V. WACHTEL, University of Bath, Department of Mathematical Sciences, UK, June 20–25.
38. S. YANCHUK, Technical University of Lodz, Division of Dynamics, Poland, April 11–22.

A.10 Academic Teaching[5]

1. Ch. Bender, *Finanzmathematik II* (lecture), Technische Universität Braunschweig, 2 SWS, Summer Semester 2005.
2. ———, *Finanzmathematik* (lecture), Technische Universität Braunschweig, 4 SWS, Winter Semester 2005/2006.
3. ———, *Finanzmathematik* (exercises), Technische Universität Braunschweig, 2 SWS, Winter Semester 2005/2006.
4. M. Birkner, *Stochastische Modelle aus der Populationsbiologie* (lecture), Technische Universität Berlin, 2 SWS, Summer Semester 2005.
5. ———, *Mathematik I für Brauerei- und Brennereitechnologen* (lecture), Technische Universität Berlin, 2 SWS, Winter Semester 2005/2006.
6. ———, *Mathematik I für Brauerei- und Brennereitechnologen* (exercises), Technische Universität Berlin, 1 SWS, Winter Semester 2005/2006.
7. A. Bovier, *Mathematische Physik III* (lecture), Technische Universität Berlin, 4 SWS, Winter Semester 2004/2005.
8. ———, *Extrema stochastischer Folgen und Prozesse* (lecture), Technische Universität Berlin, 2 SWS, Winter Semester 2005/2006.
9. A. Bovier, B. Gentz, *Stochastische Dynamik und Metastabilität* (lecture), Technische Universität Berlin, 2 SWS, Summer Semester 2005.
10. A. Bovier, B. Gentz, H. Föllmer, P. Imkeller, U. Küchler, J.-D. Deuschel, J. Gärtner, M. Scheutzow, A. Schied, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2004/2005.
11. ———, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS, 2 SWS, Summer Semester 2005.
12. ———, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Technische Universität Berlin, 2 SWS, Winter Semester 2005/2006.
13. W. Dreyer, W.H. Müller, *Grundlagen der Kontinuumsmechanik* (lecture), Technische Universität Berlin, Institut für Mechanik, 4 SWS, Winter Semester 2004/2005.
14. ———, *Projekt Nichtlineare Kontinuumsmechanik* (lecture), Technische Universität Berlin, Institut für Mechanik, 4 SWS, Summer Semester 2005.
15. K. Eppler, *Gebietsoptimierung bei elliptischen Randwertaufgaben* (lecture), Technische Universität Berlin, 2 SWS, Summer Semester 2005.
16. C. Carstensen, J. Geiser, *Diskretisierungs- und Lösungsverfahren für parabolische Differentialgleichungen: Theorie und Anwendungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2005/2006.
17. B. Gentz, *Zufällige Störungen schnell-langsamer Systeme* (lecture), Technische Universität Berlin, 2 SWS, Winter Semester 2004/2005.
18. ———, *Große Abweichungen – Theorie und Anwendungen* (lecture), Technische Universität Berlin, 2 SWS, Winter Semester 2005/2006.
19. A. Glitzky, *Mathematische Modellierung von Reaktions-Diffusionsprozessen und nichtlokalen Wechselwirkungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2004/2005.
20. ———, *Einführung in die Kontrolltheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2005/2006.

[5] SWS = semester periods per week

21. J.A. Griepentrog, *Evolutionsgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2005/2006.
22. R. Henrion, W. Römisch, M. Steinbach, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2004/2005.
23. ———, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS, Summer Semester 2005.
24. ———, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2005/2006.
25. E. Holzbecher, *Grundwassermodellierung I* (lecture), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS, Winter Semester 2005/2006.
26. ———, *Grundwassermodellierung I* (exercises), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS, Winter Semester 2005/2006.
27. D. Hömberg, *Analysis I für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS, Winter Semester 2004/2005.
28. ———, *Nichtlineare Optimierung (Optimale Bahnplanung von Industrierobotern)* (seminar), Technische Universität Berlin, 2 SWS, Summer Semester 2005.
29. ———, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS, Winter Semester 2005/2006.
30. ———, *Spieltheorie* (seminar), Technische Universität Berlin, 2 SWS, Winter Semester 2005/2006.
31. P. Mathé, *Analysis und Numerik inverser Probleme (RM/AM)* (lecture), Freie Universität Berlin, 2 SWS, Summer Semester 2005.
32. A. Mielke, *Höhere Analysis I (Funktionalanalysis)* (lecture), Humboldt-Universität zu Berlin, 4 SWS, Winter Semester 2005/2006.
33. H. Gajewski, B. Niethammer, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS, Summer Semester 2005.
34. ———, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS, Winter Semester 2005/2006.
35. V. Spokoiny, *Modern Nonparametric Modelling* (lecture), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2005/2006.
36. V. Spokoiny, W. Härdle, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2004/2005.
37. ———, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS, Summer Semester 2005.
38. ———, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2005/2006.
39. V. Spokoiny, J.G.M. Schoenmakers, *Statistische Verfahren mit Anwendungen auf Finanzmärkte* (seminar), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2004/2005.
40. ———, *Statistische Verfahren mit Anwendungen auf Finanzmärkte* (seminar), Humboldt-Universität zu Berlin, 2 SWS, Summer Semester 2005.
41. J. Sprekels, *Analysis II* (lecture), Humboldt-Universität zu Berlin, 4 SWS, Winter Semester 2004/2005.
42. ———, *Analysis III* (lecture), Humboldt-Universität zu Berlin, 4 SWS, Summer Semester 2005.
43. ———, *Analysis IV* (lecture), Humboldt-Universität zu Berlin, 4 SWS, Winter Semester 2005/2006.

44. H. Gajewski, J. Sprekels, F. Tröltzsch, R. Klein, Ch. Schütte, P. Deuflhard, R. Kornhuber, others, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS, Winter Semester 2004/2005.
45. ———, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS, Summer Semester 2005.
46. ———, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS, Winter Semester 2005/2006.
47. H. Stephan, *Einführung in die lineare Algebra* (lecture), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2004/2005.
48. ———, *Einführung in die lineare Algebra II* (lecture), Humboldt-Universität zu Berlin, 2 SWS, Summer Semester 2005.
49. ———, *Kombinatorik und Wahrscheinlichkeitstheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS, Winter Semester 2005/2006.
50. K. Tabelow, *Mathematik und Elektrotechnik* (seminar), Deutsches Herzzentrum Berlin, Akademie für Kardiotechnik, 2 SWS, Summer Semester 2005.
51. ———, *Mathematik und Elektrotechnik* (seminar), Deutsches Herzzentrum Berlin, Akademie für Kardiotechnik, 2 SWS, Winter Semester 2005/2006.
52. W. Weiss, *Kinetische Theorie* (lecture), Technische Universität Berlin, 4 SWS, Winter Semester 2004/2005.
53. K. Wilmanski, *Dynamik von mehrkomponentigen Körpern* (lecture), Technische Universität Berlin, 2 SWS, Winter Semester 2004/2005.
54. K. Wilmanski, I. Müller, P. Strehlow, W. Weiss, *Thermodynamisches Seminar* (seminar), Technische Universität Berlin/WIAS, 2 SWS, Winter Semester 2004/2005.
55. M. Wolfrum, J. Härterich, *Nichtlineare Dynamik* (senior seminar), Freie Universität Berlin/WIAS, 2 SWS, Winter Semester 2004/2005.
56. ———, *Nichtlineare Dynamik* (senior seminar), Freie Universität Berlin/WIAS, 2 SWS, Summer Semester 2005.
57. ———, *Nichtlineare Dynamik* (senior seminar), Freie Universität Berlin/WIAS, 2 SWS, Winter Semester 2005/2006.
58. L. Recke, H.-J. Wünsche, M. Wolfrum, *Mathematische Modelle der Photonik* (seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS, Summer Semester 2005.
59. ———, *Mathematische Modelle der Photonik* (seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS, Winter Semester 2005/2006.
60. K.R. Schneider, L. Recke, H.-J. Wünsche, M. Wolfrum, *Mathematische Modelle der Photonik* (seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS, Winter Semester 2004/2005.

A.11 Weierstrass Postdoctoral Fellowship Program

In 2005, the Weierstrass Institute for Applied Analysis and Stochastics has launched the *Weierstrass Postdoctoral Fellowship Program* (see http://www.wias-berlin.de/main/jobs/jobs/fellowship.html.en). The institute offers postgraduate fellowships with a duration of six up to twelve months. These fellowships are designed to enable highly-qualified young scientists to participate in the research into the mathematical problems in the fields

- Micro-, nano-, and optoelectronics
- Optimization and control of technological processes
- Phase transitions
- Stochastics in natural sciences and economics
- Flow and transport processes in continua
- Numerical methods of analysis and stochastics

and thus to further their education and training.

The fellowships can be started anytime in the year. The application deadlines are February 28 and August 31 of each year.

The first fellowship holder is Dr. Sergei Zelik, Universität Stuttgart. He started his nine-month fellowship on November 1.

A.12 Visiting Scientists[6]

A.12.1 Guests

1. I. Abnizova, Cambridge University, MRC Biostatistics Unit, Institute of Public Health, UK, December 12–23.
2. J.-P. Aguilar, Université de Toulon et du Var, Physique Mathématique Théorique, Toulon, France, April 3–16.
3. ———, May 29 – June 11.
4. M. Aizenman, Princeton University, Department of Mathematics, USA, May 5–8.
5. P. Arbenz, Eidgenössische Technische Hochschule Zürich, Institut für Wissenschaftliches Rechnen, Switzerland, September 8–11.
6. V. Arnăutu, University "Al. I. Cuza", Department of Mathematics, Iaşi, Romania, May 9 – June 6.
7. N. Berglund, CNRS Centre de Physique Théorique, Marseille, and Université de Toulon et du Var, Physique Mathématique Théorique, Toulon, France, February 1 – September 20.
8. S. Boucheron, Université Paris VII, Laboratoire de Probabilités et Modèles Aléatoires, France, May 28 – June 1.
9. A. Burmistrov, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, December 1–15.
10. C. Butucea, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, May 19–27.
11. C. Chainais-Hillairet, Université Blaise Pascal (Clermont-Ferrand 2), Laboratoire de Mathématiques Appliquées, Aubière, France, November 21–26.
12. N. Champagnat, Université Paris X, Nanterre, France, March 16–19.
13. K. Chełminski, Cardinal Stefan Wyszynski University, Faculty for Mathematics and Sciences, Warsaw, Poland, June 20 – July 18.
14. P. Colli, Università di Pavia, Dipartimento di Matematica, Italy, April 7 – May 4.
15. A. Dalalyan, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, April 4–16.
16. D. Dentcheva, Stevens Institute of Technology, Hoboken, USA, July 23–30.
17. M. Eleuteri, Università degli Studi di Trento, Dipartimento di Matematica, Povo, Italy, March 3–11.
18. P. Exner, Academy of Sciences of the Czech Republic, Nuclear Physics Institute, Prague, November 21–24.
19. R. Eymard, Université de Marne-la-Vallée, Département de Mathématiques, Champs-sur-Marne, France, October 29 – November 3.
20. A. Faggionato, Universitá "La Sapienza", Dipartimento di Matematica, Rome, Italy, March 20–25.
21. ———, November 15–20.
22. B. Fernandez, CNRS Centre de Physique Théorique, CNRS Luminy, Marseille, France, August 22 – September 23.
23. A. Foi, Tampere University of Technology, Institute of Signal Processing, Finland, April 17–24.
24. I.M. Gamba, University of Texas at Austin, Department of Mathematics, USA, September 20–25.

[6] Only stays of more than three days are listed.

25. P. Gapeev, Russian Academy of Sciences, Institute of Control Sciences, Moscow, October 17 – December 17.
26. M.E. Glicksmann, Materials Science & Engineering, Rensselaer Polytechnic Institute, Troy, USA, November 25–28.
27. E. Gobet, Centre de Mathématiques Appliquées, École Polytechnique, Palaiseau, France, January 24–29.
28. Y. Golubev, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, November 2–30.
29. I. Grama, Université de Bretagne Sud, Laboratoire SABRES, Vannes, France, October 24–31.
30. R.B. Guenther, Oregon State University, Mathematics Department, Corvallis, USA, August 21 – September 3.
31. A. Heubner, Fraunhofer-Institut für Integrierte Systeme und Bauelementetechnologie, Erlangen, May 8–11.
32. J. Horowitz, Northwestern University, Weinberg College of Arts and Sciences, Department of Economics, Evanston, USA, October 8–15.
33. I. Ignatiouk, Université de Cergy-Pontoise, Département de Mathématiques, France, April 25–29.
34. D. Ioffe, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, July 25 – August 25.
35. V. Katkovnik, Tampere University of Technology, Institute of Signal Processing, Finland, April 17–24.
36. S. Kim, University of Tokyo, Graduate School of Mathematical Sciences, Japan, September 11–27.
37. D. Kourounis, University of Ioannina, Department of Material Science, Greece, September 26 – December 23.
38. T. Kozoubskaya, Russian Academy of Sciences, Institute for Mathematical Modelling, Computational Aeroacoustics Laboratory, Moscow, December 8–23.
39. V. Kozyakin, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, January 3 – February 3.
40. R. Krämer, Technische Universität Chemnitz, Fakultät für Mathematik, May 30 – June 3.
41. Ch. Kühn, Johann-Wolfgang-Goethe-Universität Frankfurt, Fachbereich Mathematik, Frankfurt/Main, June 6–9.
42. K. Kuhnen, Universität des Saarlandes, Lehrstuhl für Prozessautomatisierung, Saarbrücken, February 20 – March 20.
43. O. Kurbanmuradov, Turkmen State University, Physics and Mathematics Research Center, Ashkhabat, April 16 – June 18.
44. ———, September 24 – December 24.
45. Ch.J. Larsen, University of Warwick, Mathematics Institute, UK, November 7–11.
46. P. Laurençot, UFR MIG, Mathématiques pour l'Industrie et la Physique, Université Paul Sabatier Toulouse, France, April 22–30.
47. O. Lepski, Université de Provence, Centre de Mathématiques et d'Informatique, Marseille, France, October 24–30.
48. A. Levykin, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, February 20 – March 20.
49. ———, September 24 – December 24.
50. A. Linke, DFG Research Center Matheon, Berlin, January 1 – December 31.

51. A. Loyer, Université de Toulon et du Var, Physique Mathématique Théorique, Toulon, France, April 25 – June 25.
52. M.M. Malamud, Donetsk National University, Department of Mathematics, Ukraine, December 12–15.
53. M. Marchenko, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, September 25 – December 11.
54. M. Mascagni, The Florida State University, Department of Computer Science, Tallahassee, USA, October 16–19.
55. R. Messikh, EURANDOM, Eindhoven, The Netherlands, January 16–21.
56. G.N. Milstein, Ural State University, Department of Mathematics, Ekaterinburg, Russia, November 15, 2004 – April 15, 2005.
57. P. Mörters, University of Bath, Department of Mathematical Sciences, UK, March 19–25.
58. ———, August 7–25.
59. ———, December 11–23.
60. O. Muscato, University of Catania, Department of Mathematics and Informatics, Italy, August 21–28.
61. S. Nagaev, Steklov Institute of Mathematics, Novosibirsk, Russia, June 6–17.
62. M. Nizette, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, December 4–16.
63. A. Oron, Technion — Israel Institute of Technology, Faculty of Mechanical Engineering, Haifa, July 8–27.
64. C. Patz, CERMICS, Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée, France, October 30 – November 11.
65. ———, November 28 – December 13.
66. S.V. Pereverzev, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, May 1–31.
67. M. Pietrzyk, Warsaw University of Technology, Poland, April 24–30.
68. B. Plamenevskij, St. Petersburg State University, Department of Mathematical Physics, Russia, October 1–31.
69. K. Pyragas, Semiconductor Physics Institute, Vilnius, Lithuania, May 24–28.
70. J. Rademacher, University of British Columbia, Pacific Institute for the Mathematical Sciences, Vancouver, Canada, January 17 – February 11.
71. P. Rigollet, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, June 27 – July 3.
72. L. Ringstadt-Olsen, University of Tromsø, Department of Mathematics and Statistics, Norway, November 22 – December 21.
73. E. Rocca, Università degli Studi di Milano, Dipartimento di Matematica "Federigo Enriques", Italy, November 22 – December 15.
74. Ch. Rohde, Universität Bielefeld, Fakultät für Mathematik, March 20–25.
75. R. Rossi, Università degli Studi di Brescia, Dipartimento di Matematica, Italy, November 28 – December 4.
76. ———, December 4–10.
77. A. Ruszczynski, Rutgers University, Rutgers Center for Operations Research, Piscataway, USA, July 23–30.
78. O. Schenk, Universität Basel, Fachbereich Informatik, Switzerland, August 7–28.
79. F. Schilder, University of Bristol, Department of Engineering Mathematics, UK, December 19–22.
80. F. Schmid, Universität Stuttgart, Fachbereich Mathematik, Institut für Analysis, Dynamik und Modellierung, May 11–14.

81. U. Schmock, Vienna University of Technology, Financial and Actuarial Mathematics, Institute for Mathematical Methods in Economics, Austria, June 6–9.
82. M. Schweizer, Eidgenössische Technische Hochschule Zürich, Institut für Mathematik, Switzerland, February 23–27.
83. A. Seeger, Université d'Avignon, Département de Mathématiques, France, April 6–28.
84. I. Shalimova, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, April 30 – May 30.
85. ———, September 24 – October 21.
86. ———, November 18 – December 18.
87. S. Sheshenin, Moscow State University, Institute of Mechanical Mathematics, Russia, July 10–14.
88. J. Shewchuk, University of California at Berkeley, Computer Science Division, USA, September 24 – October 23.
89. J. Sieber, University of Bristol, Department of Engineering Mathematics, UK, May 1–11.
90. ———, August 16 – September 4.
91. J. Sokołowski, Université de Nancy I, Laboratoire de Mathématiques, Vandœuvre-lès-Nancy, France, August 6–13.
92. T. Sottinen, University of Helsinki, Department of Mathematics and Statistics, Finland, August 27 – September 4.
93. Ch. Sparber, Wolfgang Pauli Institut & Fakultät für Mathematik, Universität Wien, Austria, October 10–15.
94. S. Sperlich, Universidad Carlos III de Madrid, Departamento de Estadística y Econometría, Spain, December 15, 2004 – January 22, 2005.
95. ———, December 21, 2005 – January 20, 2006.
96. K. Staliunas, Universitat Politecnica de Catalunya, Departament de Fisica i Enginyeria Nuclear, Barcelona, Spain, October 26 – November 2.
97. C. Starica, Chalmers University of Technology, Department of Mathematical Statistics, Gothenburg, Sweden, February 6–12.
98. U. Stefanelli, Istituto di Matematica Applicata e Tecnologie Informatiche, Pavia, Italy, June 19–24.
99. C. Strugarek, Electricité de France R&D, Clamart, November 20 – December 5.
100. P. Tankov, Institut National de Recherche en Informatique et en Automatique, Le Chesnay, France, June 26 – July 3.
101. U. Tautenhahn, Hochschule Zittau/Görlitz, Fachbereich Mathematik/Naturwissenschaften, Zittau, July 18–22.
102. D. Tiba, Romanian Academy, Institute of Mathematics, Bucharest, March 1–31.
103. A. Timofte, Universität Stuttgart, Fachbereich Mathematik, Institut für Analysis, Dynamik und Modellierung, April 25 – August 31.
104. M. Tlidi, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, June 17 – July 7.
105. B. Tollkühn, Fraunhofer-Institut für Integrierte Systeme und Bauelementetechnologie, Erlangen, May 8–11.
106. M. Tretyakov, University of Leicester, Department of Mathematics, UK, March 20 – April 13.
107. D. Turaev, Ben Gurion University of the Negev, Department of Mathematics, Beer Sheva, Israel, January 16–23.
108. ———, July 9–25.

109. ———, August 1–12.
110. S. VAN BELLEGEM, Université Catholique de Louvain, Institut de Statistique, Louvain-la-Neuve, Belgium, May 9–20.
111. V.A. VATUTIN, Steklov Institute of Mathematics, Moscow, Russia, November 10 – December 10.
112. S. VERDUYN LUNEL, University of Leiden, Mathematical Institut, The Netherlands, May 25–28.
113. A. VERETENNIKOV, University of Leeds, Department of Statistics, UK, June 7–18.
114. C. VIAL, Université Paris X, Laboratoire Modal'X, Nanterre, France, May 15–27.
115. E.A. VIKTOROV, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, May 25–28.
116. A. VISINTIN, Università di Trento, Dipartimento di Matematica, Italy, December 3–8.
117. H. VOSS, Weill Medical College of Cornell University, Citigroup Biomedical Imaging Center, New York, USA, June 26 – July 3.
118. Y. WANG, University of Tokyo, Graduate School of Mathematical Sciences, Japan, September 22–28.
119. G. WARNECKE, Otto-von-Guericke-Universität Magdeburg, Institut für Analysis und Numerik, February 22 – March 4.
120. ———, March 14–18.
121. M. YAMAMOTO, University of Tokyo, Department of Mathematical Sciences, Japan, March 17–29.
122. ———, September 10–28.
123. Q. YAO, London School of Economics, Department of Statistics, UK, July 3–11.
124. V.A. ZAGREBNOV, Université Aix-Marseille II, Centre de Physique Théorique, France, August 29 – September 18.
125. I. ZÄHLE, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, May 23–27.
126. ———, September 26–30.
127. D. ZEITZ, Alstom Power AG, Baden, Switzerland, July 10–31.
128. S. ZHANG, Eindhoven University of Technology, COBRA Research Institute, The Netherlands, November 13–18.
129. H. ZHAO, DFG Research Center MATHEON, Berlin, June 15 – December 31.
130. S. ZHENG, Fudan University, Institute of Mathematics, Shanghai, China, November 26 – December 4.

A.12.2 Scholarship Holders

1. J. BONDARENKO, Universität der Bundeswehr Hamburg, Fachbereich für Wirtschafts- und Organisationswissenschaften, DAAD Fellowship, August 15 – October 15.
2. I. BOROVSKAYA, Russian Academy of Sciences, Institute for Mathematical Modelling, Moscow, DAAD Fellowship, October 1, 2005 – March 31, 2006.
3. C.-G. LEFTER, University of Iaşi, Department of Mathematics, Romania, Humboldt Research Fellowship, May 1, 2005 – April 30, 2006.
4. A. MÜNCH, Humboldt-Universität zu Berlin, Institut für Mathematik, Heisenberg Fellowship of the Deutsche Forschungsgemeinschaft (German Research Foundation), November 1, 2003 – October 31, 2006.
5. T. ROUBÍČEK, Charles University, Mathematical Institute, Prague, Czech Republic, Humboldt Research Fellowship, June 1–30.
6. Y. XIA, National University of Singapore, Department of Statistics I, Humboldt Research Fellowship, July 11 – August 11.
7. S. ZELIK, Universität Stuttgart, Institut für Analysis, Dynamik und Modellierung, Lehrstuhl für Analysis und Modellierung, Stuttgart, Weierstrass Postdoctoral Fellowship Program, November 1, 2005 – July 31, 2006.

A.12.3 Doctoral Candidates and Post-docs supervised by WIAS Collaborators

1. M. AN DER HEIDEN, Technische Universität Berlin, Graduate College "Stochastic Processes and Probabilistic Analysis", doctoral candidate, since May 1, 2002.
2. A. DEPPERSCHMIDT, Technische Universität Berlin, doctoral candidate, since January 1, 2004.
3. A. KLIMOVSKI, Technische Universität Berlin, Graduate College "Stochastic Processes and Probabilistic Analysis", doctoral candidate, since June 1, 2003.
4. A. MAINIK, Universität Stuttgart, Institut für Analysis, Dynamik und Modellierung, Collaborative Research Center SFB 404 "Multifield Problems", doctoral candidate, since February 1.
5. C. PATZ, Universität Stuttgart, Institut für Analysis, Dynamik und Modellierung, doctoral candidate, since January 1.
6. F. SCHMID, Universität Stuttgart, Institut für Analysis, Dynamik und Modellierung, doctoral candidate, since January 1.
7. A. TIMOFTE, Universität Stuttgart, Institut für Analysis, Dynamik und Modellierung, European Union "Smart Systems: New Materials, Adaptive Systems and their Nonlinearities. Modelling, Control and Numerical Simulation", doctoral candidate, January 1 – August 31.

A.13 Guest Talks

1. M. Adams, University of Essex, Department of Electronic Systems Engineering, Colchester, UK, *Optically injected semiconductor lasers for network transmission and switching*, November 24.
2. M. Aizenman, Princeton University, Department of Mathematics, USA, *On the stability of the ac spectra of tree graph operators under weak disorder*, May 6.
3. P. Arbenz, Eidgenössische Technische Hochschule Zürich, Institut für Wissenschaftliches Rechnen, Switzerland, *On a parallel multilevel preconditioned Maxwell eigensolver*, September 8.
4. V. Arnăutu, University "Al. I. Cuza", Department of Mathematics, Iaşi, Romania, *On the analysis of age-dependent population dynamics*, June 2.
5. S. Boucheron, Université Paris VII, Laboratoire de Probabilités et Modèles Aléatoires, France, *Some concentration inequalities and their applications to minimum contrast estimation*, June 1.
6. E. Burman, Ecole Polytechnique Fédérale de Lausanne, Faculté de Mathématiques, Switzerland, *Interior penalty procedures for transport problems: Asymptotic limits and monotonicity*, December 8.
7. C. Butucea, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, *Estimation of the Wigner function in quantum homodyne tomography with noisy data*, May 25.
8. C. Chainais-Hillairet, Université Blaise Pascal (Clermont-Ferrand 2), Laboratoire de Mathématiques Appliquées, Aubière, France, *Reconstruction of gradients in finite volume scheme. Application to the discretization of the Joule heating term*, November 24.
9. N. Champagnat, Université Paris X, Nanterre, France, *A microscoping interpretation for a Markov jump process of evolution*, March 17.
10. K. Chełminski, Cardinal Stefan Wyszynski University, Faculty for Mathematics and Sciences, Warsaw, Poland, *Quasistatische Probleme in der Theorie nichtelastischer Deformationen*, July 14.
11. P. Colli, Università di Pavia, Dipartimento di Matematica, Italy, *Existence and large time behavior for an entropy balance and linear thermal memory model for phase transitions*, April 27.
12. A. Dalalyan, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, *Semiparametric estimation of the shift: Second order efficiency*, April 13.
13. D. Dentcheva, Stevens Institute of Technology, Department of Mathematical Sciences, Hoboken, USA, *Risk averse optimization*, July 26.
14. S. El Manouni, University of Fez, Morocco, *Existence and regularity of solutions for some nonlinear elliptic equations involving the p-Laplacian*, January 19.
15. M. Eleuteri, Università degli Studi di Trento, Dipartimento di Matematica, Povo, Italy, *Some classes of parabolic PDEs with hysteresis*, March 4.
16. H. Emmerich, RWTH Aachen, Institut für Gesteinshüttenkunde, *Mikro-Makro-Simulationen peritektischer Erstarrung*, May 3.
17. P. Exner, Academy of Sciences of the Czech Republic, Nuclear Physics Institute, Prague, *Resonance effects in transport through leaky graphs*, November 23.
18. R. Eymard, Université de Marne-la-Vallée, Département de Mathématiques, Champs-sur-Marne, France, *Finite volume schemes for anisotropic diffusion operators*, November 3.
19. F. Falk, Institut für Physikalische Hochtechnologie Jena, *Laserkristallisation von Halbleitern*, April 8.
20. E. Feireisl, Academy of Sciences of the Czech Republic, Mathematical Institute, Prague, *On some singular limits for the full Navier–Stokes–Fourier system*, October 26.
21. K. Fraedrich, Universität Hamburg, Meteorologisches Institut, *tba*, November 21.
22. R. Giese, Gaswärme-Institut Essen, *Energetische Optimierung von Thermoprozessanlagen*, June 13.

23. M.E. Glicksmann, Materials Science & Engineering, Rensselaer Polytechnic Institute, Troy, USA, *How studying melting may explain freezing*, September 27.
24. E. Gobet, Centre de Mathématiques Appliquées, École Polytechnique, Palaiseau, France, *Backward stochastic differential equations in finance: A resolution via a regression-based Monte Carlo method*, January 28.
25. Y. Golubev, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, *The method of risk envelopes and oracle inequalities*, November 9.
26. E. Grigorieva, International A. Sakharov Environmental University, Department of Physics, Minsk, Belarus, *Order parameters for class-B lasers with a long-time delayed feedback*, July 21.
27. R.B. Guenther, Oregon State University, Mathematics Department, Corvallis, USA, *The Navier–Stokes' equations: Their derivation, linearization, and solution of the linear problems*, August 30.
28. J. Härterich, Freie Universität Berlin, Institut für Mathematik I, *Front motion in viscous conservation laws with stiff source terms*, November 8.
29. B. Heinemann, IHP, Frankfurt (Oder), *Technologiebausteine für Kommunikationssysteme, integriert auf einem Chip*, November 9.
30. G. Huyet, University College Cork, Physics Department, Ireland, *Dynamics of semiconductor lasers*, July 11.
31. I. Ignatiouk, Université de Cergy-Pontoise, Département de Mathématiques, France, *On the spectrum of Markov semigroups via sample path large deviations*, April 27.
32. K. Jacobs, Universität des Saarlandes, FR Experimentalphysik, *Dynamik von Flüssigkeiten in der Nähe einer Grenzfläche: Eine experimentelle Sicht*, July 25.
33. V. Katkovnik, A. Foi, Tampere University of Technology, Institute of Signal Processing, Finland, *Spatially adaptive local likelihood approximations for direct and indirect observations*, April 20.
34. D. Kourounis, University of Ioannina, Department of Material Science, Greece, *The FEM-FCT stabilization method for convection dominated problems*, October 6.
35. H. Kozono, Tohoku University, Mathematical Institute, Sendai, Japan, *Some variational inequality of vector fields and its application to the Helmholtz–Weyl decomposition in L^r*, November 23.
36. V. Kozyakin, Russian Academy of Sciences, Institute for Information Transmission Problems, Moscow, Russia, *Asynchronous systems: A short survey and problems*, January 25.
37. R. Krämer, Technische Universität Chemnitz, Fakultät für Mathematik, *A two step approach for parameter estimation in a generalized bivariate Ornstein–Uhlenbeck model*, May 31.
38. Ch. Kühn, Johann-Wolfgang-Goethe-Universität Frankfurt, Fachbereich Mathematik, Frankfurt/Main, *Convertible bonds in jump-diffusion models*, June 8.
39. N. Kutz, University of Washington, Department of Mathematics, USA, *Mode-locked soliton lasers*, September 5.
40. Ch.J. Larsen, University of Warwick, Mathematics Institute, UK, *Some problems in the modeling and analysis of quasi-static evolution in brittle fracture*, November 10.
41. P. Laurençot, UFR MIG, Mathématiques pour l'Industrie et la Physique, Université Paul Sabatier Toulouse, France, *Mass conserving self-similar solutions to the Smoluchowski coagulation equation*, April 27.
42. C.-G. Lefter, University of Iaşi, Department of Mathematics, Romania, *Controllability and stabilization of parabolic equations and systems*, May 31.
43. K. Lu, Brigham Young University, Department of Mathematics, Provo, USA, *Invariant manifolds for infinite-dimensional dynamical systems*, October 25.
44. P. Maass, Universität Bremen, Zentrum für Technomathematik, *Wavelets in der Datenanalyse — von Finanzdaten bis zur Windmessung*, May 9.

45. Y. Maistrenko, B. Lysyansky, Forschungszentrum Jülich, Medizinisches Institut, *Complex dynamics in a system of two coupled phase oscillators with delay*, December 6.
46. M.M. Malamud, Donetsk National University, Department of Mathematics, Ukraine, *A generalization of the Aronszajn–Donoghue theory*, December 14.
47. M. Mascagni, The Florida State University, Department of Computer Science, Tallahassee, USA, *Stochastic simulation in biological electrostatics*, October 17.
48. D. McDonald, University of Ottawa, Department of Mathematics and Statistics, Canada, *Mean field convergence of a rate model of multiple TCP connections through a buffer implementing RED*, April 27.
49. Ch. Melcher, Humboldt-Universität zu Berlin, Institut für Mathematik, *Motion of magnetic domain walls*, January 11.
50. D. Michaelis, Fraunhofer-Institut für Angewandte Optik und Feinmechanik, Jena, *Raum-zeitliche Dynamik in nichtlinear-optischen Systemen*, July 15.
51. M. Mönster, Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Abteilung C2, Berlin, *Soliton mode-locked Nd-doped microstructured fiber laser*, July 1.
52. C. Monthus, Service de Physique Théorique, CEA/SPhT, Gif-sur-Yvette, France, *Random walks in random media: Localization and ageing properties*, February 16.
53. N. Nefedov, Moscow State University, Faculty of Physics, Russia, *On moving fronts in periodically forced reaction-diffusion systems*, November 29.
54. M. Nizette, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, *Instabilities in semiconductor lasers with filtered optical feedback: An analytical study*, December 8.
55. ———, *Pulse interaction via gain and loss dynamics in passive mode-locking*, December 13.
56. A. Oron, Technion — Israel Institute of Technology, Faculty of Mechanical Engineering, Haifa, *Marangoni instability in binary liquids with Soret effect*, July 26.
57. L. Overbeck, HypoVereinsbank/Justus-Liebig-Universität Gießen, *Valuation of structured credit products*, June 6.
58. U. Parlitz, Universität Göttingen, Drittes Physikalisches Institut, *Kontrolle und Synchronisation chaotischer Laserdynamik*, June 3.
59. C. Patz, CERMICS, Ecole Nationale des Ponts et Chaussées, Marne-la-Vallée, France, *Dispersive behavior in harmonic oscillator chains*, November 2.
60. R.P. Pego, Carnegie-Mellon University, Pittsburgh, USA, *Divorcing pressure from viscosity in incompressible Navier–Stokes dynamics*, June 15.
61. S.V. Pereverzev, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, *Regularization in Hilbert scales under general smoothing conditions*, May 18.
62. T. Perez, Universitat de les Illes Balears, Physics Department, Palma de Mallorca, Spain, *Chaos synchronization: Applications to data encryption*, June 23.
63. V. Petzet, Universität Bayreuth, Lehrstuhl für Ingenieurmathematik, *Verhinderung der Heißrissbildung beim Mehrstrahl-Laserschweißen durch Optimierung*, January 11.
64. B. Plamenevskij, St. Petersburg State University, Department of Mathematical Physics, Russia, *Scattering and electron transport in quantum wires*, October 19.
65. ———, *Elastodynamics in domains with edges*, October 25.
66. U. Prahl, RWTH Aachen, Institut für Eisenhüttenkunde, *Prozesskettenmodellierung in der Warmumformung*, July 15.
67. K. Pyragas, Semiconductor Physics Institute, Vilnius, Lithuania, *Delayed feedback control technique and its analytical treatment at a Hopf bifurcation*, May 27.

68. E.R. Racec, Brandenburgische Technische Universität Cottbus, *Transport properties of a single electron transistor*, April 13.
69. P. Racec, IHP/BTU JointLab Cottbus, *Application of R-matrix formalism in modeling of semiconductor nanostructures*, January 12.
70. J. Rademacher, Pacific Institute of the Mathematical Sciences, University of British Columbia, Vancouver, Canada, *The absolute spectrum of wave trains*, January 25.
71. R. Ramlau, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, *Inverse Unwuchtkontrolle zum Online-Monitoring von Windenergieanlagen*, November 28.
72. L. Recke, Humboldt-Universität zu Berlin, Institut für Mathematik, *On eigenvalues and stability related to the travelling wave model*, June 9.
73. ———, *Über semilineare hyperbolische Randanfangswertprobleme mit unstetigen Koeffizienten*, November 9.
74. P. Rigollet, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, *Block Stein and aggregation for density estimators*, June 29.
75. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, *Ionized incompressible fluid mixtures*, June 8.
76. A. Ruszczynski, Rutgers University, Rutgers Center for Operations Research (RUTCOR), Piscataway, USA, *Optimization under stochastic dominance constraints*, July 26.
77. O. Schenk, Universität Basel, Fachbereich Informatik, Switzerland, *On large scale diagonalization techniques for the Anderson model of localization*, August 25.
78. F. Schilder, University of Bristol, Department of Engineering Mathematics, UK, *Computing Arnol'd tongue scenarios*, December 20.
79. B. Schmalfuss, Universität Paderborn, Fakultät für Elektrotechnik, Informatik und Mathematik, *Mittelungsmethoden bei zufälligen dynamischen Systemen*, March 29.
80. U. Schmock, Vienna University of Technology, Financial and Actuarial Mathematics, Institute for Mathematical Methods in Economics, Austria, *Models for dependent credit risks and their calibration*, June 8.
81. H.-J. Schwarzmaier, Klinikum Krefeld, *Grundlagen der laserinduzierten, interstitiellen Thermotherapie*, January 24.
82. A. Seeger, Université d'Avignon, Département de Mathématiques, France, *Exponentiation of multivalued maps and reachable sets of differential inclusions*, April 26.
83. G. Sell, University of Minnesota, School of Mathematics, Minneapolis, USA, *What longtime dynamics tell us about building good models of the climate*, May 24.
84. S. Sheshenin, Moscow State University, Institute of Mechanical Mathematics, Russia, *Homogenization of thin solids: Theory and application to rubber-cord belt and stamped plate*, July 12.
85. J. Shewchuk, University of California at Berkeley, Computer Science Division, USA, *Star splaying: An algorithm for repairing nearly-Delaunay triangulations*, October 14.
86. J. Sieber, University of Bristol, Department of Engineering Mathematics, UK, *Continuation using time-delayed feedback control — First progress report*, September 1.
87. S. Siltanen, Global X-ray, GE Healthcare, Tuusula, Finland, *Low dose three-dimensional medical X-ray imaging*, October 31.
88. J. Sokołowski, Université de Nancy I, Laboratoire de Mathématiques, Vandœuvre-lès-Nancy, France, *Modelling of topological derivatives for contact problems*, August 10.
89. Ch. Sparber, Wolfgang Pauli Institut & Fakultät für Mathematik, Universität Wien, Austria, *Asymptotic regimes for nonlinear Schrödinger equations in periodic potentials*, October 12.

90. K. Staliunas, Universitat Politecnica de Catalunya, Departament de Fisica i Enginyeria Nuclear, Barcelona, Spain, *Nondiffractive light in photonic crystals*, October 27.
91. E. Stepanov, Università di Pisa, Dipartimento di Matematica, Italy, *Invariant measures for a class of generalized stochastic dynamical systems*, February 10.
92. I. Straškraba, Academy of Sciences of the Czech Republic, Mathematical Institute, Prague, *Lyapunov functional for Navier–Stokes equations*, August 15.
93. H. Struchtrup, University of Victoria, Department of Mechanical Engineering, Canada, *A macroscopic transport model for PEM membranes based on the microscale behavior*, August 4.
94. C. Strugarek, Electricité de France R&D, Clamart, France, *Stochastic optimization: New discretization schemes and decomposition issues*, November 29.
95. I. Sushko, Università degli Studi di Urbino, Istituto di Scienze Economiche, Italy, *Border-collision bifurcation curves for a family of unimodal piecewise smooth maps*, August 25.
96. M. Tretyakov, University of Leicester, Department of Mathematics, UK, *Numerical algorithms for forward-backward stochastic differential equations*, April 12.
97. D. Turaev, Ben Gurion University of the Negev, Department of Mathematics, Beer Sheva, Israel, *On Hausdorff dimension of nonuniformly hyperbolic sets*, January 18.
98. H. Uecker, Universität Karlsruhe, Fakultät für Mathematik, *Justification of the nonlinear Schrödinger equation in spatially periodic media*, June 3.
99. S. van Bellegem, Université Catholique de Louvain, Institut de Statistique, Louvain-la-Neuve, Belgium, *Semiparametric estimation by model selection for locally stationary processes*, May 11.
100. M. Väth, Freie Universität Berlin, Institut für Mathematik I, *Degree and global bifurcation for elliptic equations with multivalued unilateral conditions*, June 14.
101. S. Verduyn Lunel, University of Leiden, Mathematical Institute, The Netherlands, *Completeness of spaces spanned by eigenfunctions*, May 26.
102. ———, *The role of the essential spectrum in delayed feedback control*, May 27.
103. E. Viktorov, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, *Dynamics of two-state quantum dot lasers*, May 26.
104. H. Voss, Citigroup Biomedical Imaging Center, Weill Medical College of Cornell University, Ithaka, USA, *Understanding functional connectivity of the brain: Diffusion tensor magnetic resonance imaging*, June 27.
105. H. Wenzel, Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin, *Higher order Bragg waveguide gratings — Theory and experiment*, December 1.
106. H. Wöhler, autronic-MELCHERS GmbH Karlsruhe, *Modellierung und Simulation von LCDs*, April 25.
107. J. Wolf, Humboldt-Universität zu Berlin, *Energie-Gleichung für blow-up Lösungen der Euler-Gleichungen*, February 9.
108. U. Wulf, Brandenburgische Technische Universität Cottbus, *Resonanter Transport in Halbleiterquantenstrukturen*, April 20.
109. M. Yamamoto, University of Tokyo, Department of Mathematical Sciences, Japan, *Determination of Lamé coefficients in plate equations with nonhomogeneous materials*, September 22.
110. Q. Yao, London School of Economics, Department of Statistics, UK, *Modelling multivariate volatilities via conditionally uncorrelated components*, July 6.
111. V.A. Zagrebnov, Université Aix-Marseille II, Centre de Physique Théorique, France, *Superradiant Bose–Einstein condensation*, September 15.
112. I. Zähle, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, *Genealogies in the stepping stone model*, May 25.

113. M. Zaks, Humboldt-Universität zu Berlin, Institut für Physik, *Dynamics in noise-driven ensembles of globally coupled excitable systems*, February 15.

114. S. Zhang, Eindhoven University of Technology, COBRA Research Institute, The Netherlands, *Multiple state flip-flop optical memory based on strongly coupled oscillators*, November 17.

A.14 Software

AWS (contact: J. Polzehl, phone: +49 30/20372-481)

AWS is an **A**daptive **W**eights **S**moothing package. A reference implementation of the adaptive weights smoothing procedures (AWS) is available in form of a contributed package of the R-Project for Statistical Computing (http://www.r-project.org/).

The package includes functions for local polynomial structural adaptive smoothing in regression models with additive errors and for local constant structural adaptive smoothing in exponential family models, the latter including binary response, Poisson regression, exponential regression, and volatility models. The special case of a grid design allows for efficient reconstruction of non-smooth images in 2D and 3D.

The package can be obtained from http://CRAN.R-project.org/.

An extension of this package currently allows for multivariate models and contains functions for the analysis of fMRI and dMRI data.

BOP (contact: J. Borchardt, phone: +49 30/20372-485)

The simulator BOP (**B**lock **O**rientend **P**rocess simulator) is a software package for large-scale process simulation. It allows to solve dynamic as well as steady-state problems and enables Monte Carlo simulations. Due to an equation-based approach, a wide range of processes as they occur in chemical process industries or other process engineering environments can be simulated.

The modeling language of BOP is a high-level language that supports a hierarchically unit-oriented description of the process model and enables a simulation concept that is based on a divide-and-conquer strategy. Exploiting this hierarchical modeling structure, the generated system of coupled differential and algebraic equations (DAEs) is partitioned into blocks, which can be treated almost concurrently. The numerical methods used are especially adopted for solving large-scale problems on parallel computers. They include backward differentiation formulae (BDF), block-structured Newton-type methods, and sparse matrix techniques.

BOP is implemented under UNIX on parallel computers with shared memory (Cray J90, SGI Origin2000, Compaq AlphaServer), but can also be run on different single processor machines, as well as under Windows XP on PCs. So far it has been successfully used for the simulation of several real-life processes in heat-integrated distillation, sewage sludge combustion, or catalytic CO oxidation in automotive oxygen sensors, for example. Currently, it is commercially used for gas turbine simulation.

Detailed information: http://www.wias-berlin.de/software/BOP

ClusCorr98® (contact: H.-J. Mucha, phone: +49 30/20372-573)

The statistical software ClusCorr98® is an interactive statistical computing environment with the main focus on clustering techniques. A highlight is the automatic validation technique of cluster analysis results performed by a general built-in validation tool that is based on resampling techniques. For example, the automatic validation of hierarchical clustering can be considered as a three-level assessment of stability. The first and most general level is decision-making about the appropriate number of clusters. The decision is based on such well-known measures of correspondence between partitions like the Rand index, the adjusted Rand index, and the index of Fowlkes and Mallows. Second, the stability of each individual cluster is assessed based on measures of similarity between sets, e.g., the asymmetric measure of cluster agreement or the symmetric Jaccard measure. It does makes sense to investigate the (often quite different) specific stability of clusters.

In the third and most detailed level of validation, the reliability of the cluster membership of each individual observation can be assessed.

ClusCorr98® performs exploratory data analysis mainly by using adaptive methods of cluster analysis, classification, and multivariate visualization. The main focus here is on simple stable models accompanied by appropriate multivariate (graphical) methods like principal components plots and informative dendrograms (binary trees). Usually, the performance and stability of these methods can be improved by using them in a local and adaptive local fashion.

ClusCorr98® uses the Excel spreadsheet environment and its database connectivity. The programming language is Visual Basic for Applications (VBA).

Further information: http://www.wias-berlin.de/software/ClusCorr98 and
http://www.wias-berlin.de/people/mucha/Clustering

DiPoG (contact: A. Rathsfeld, phone: +49 30/20372-457)

The program package DiPoG (**D**irect and **i**nverse **P**roblems for **o**ptical **G**ratings) provides simulation and optimization tools for periodic diffractive structures with multilayer stacks.

The direct solver computes the field distributions and efficiencies of given gratings for TE and TM polarization as well as under conical mounting for arbitrary polygonal surface profiles. The inverse solver deals with the optimal design of gratings, realizing given optical functions, for example, far-field patterns, efficiency, or phase profiles. The algorithms are based on coupled generalized finite/boundary elements and gradient-type optimization methods.

For detailed information please see http://www.wias-berlin.de/software/DIPOG.

gltools (contact: J. Fuhrmann, phone: +49 30/20372-560)

gltools has been designed with the needs of numerical analysts in mind. Thus, unlike many other packages available, it can be used to enhance existing codes with interactive or non-interactive graphical output. It enhances the OpenGL API with additional functionality allowing to use it for the efficient visualization of time-dependent data on one-, two-, and three-dimensional simplicial grids. Recently, a graphical user interface based on the FLTK toolkit has been added to the package.

Please find further information under http://www.wias-berlin.de/software/gltools.

LDSL-tool (contact: M. Radziunas, phone: +49 30/20372-441)

LDSL-tool (**L**ongitudinal **D**ynamics in **S**emiconductor **L**asers) is a tool for the simulation and analysis of the nonlinear longitudinal dynamics in multi-section semiconductor lasers. This software is used to investigate and to design lasers that exhibit various nonlinear effects such as self-pulsations, chaos, hysteresis, mode switching, excitability, and synchronization to an external signal frequency.

LDSL-tool combines models of different complexity, ranging from partial differential equation (PDE) to ordinary differential equation (ODE) systems. A mode analysis of the PDE system, a comparison of the different models, and a numerical bifurcation analysis of PDE systems are also possible.

Detailed information: http://www.wias-berlin.de/software/ldsl

pdelib (contact: J. Fuhrmann, phone: +49 30/20372-560)

`pdelib` is a collection of software components that are useful to create simulators based on partial differential equations. The main idea of the package is modularity, based on a bottom-up design realized in the C++ programming language. Among others, it provides libraries for

- iterative solvers
- sparse matrix structures with preconditioners and direct solver interfaces
- simplex grid handling
- parallelization on SMP architectures
- graphical output using `gltools` and OpenGL
- user interface based on the scripting language Lua
- graphical user interface based on the FLTK toolkit

Further, based on the finite volume implicit Euler method, a solver for systems of nonlinear reaction-diffusion-convection equations in heterogeneous one-, two-, and three-dimensional domains has been implemented that is part of the package.

For more information please see also http://www.wias-berlin.de/software/pdelib.

WIAS-HiTNIHS (contact: O. Klein, phone: +49 30/20372-533)

The WIAS-**Hi**gh **T**emperature **N**umerical **I**nduction **H**eating **S**imulator constitutes a transient simulation tool for the temperature evolution in axisymmetric technical systems that are subject to intense heating by induction. The simulator accounts for heat transfer by radiation through cavities, and it allows for changes in the material parameters due to the rising temperature and for some kinds of anisotropy within the thermal conductivity.

The simulator is designed to deal with complicated axisymmetric setups having a polygonal 2D projection. The software is based on the WIAS program package `pdelib` for the numerical solution of partial differential equations and has a graphical user interface provided by `WIAS-MatConE`.

`WIAS-HiTNIHS` has been and is further developed within the project *"Numerical simulation and optimization of SiC single crystal growth by sublimation from the gas phase"* supported by BMBF (until 2003) and DFG (since 2002).

Please find further information under http://www.wias-berlin.de/software/hitnihs.

WIAS-MatConE (contact: Olaf Klein, phone: +49 30/20372-533)

The WIAS-**Mat**erial data file and **Con**trol file **E**dit GUI is a software tool to provide prototypical graphical user interfaces (GUIs) for creating and editing files that are used as inputs for simulation software, like, for example, material data and control files.

The contents of a file type to be considered are described by a list of input requests for real numbers, integer numbers, strings, file names, fields of real numbers, and fields of real vectors, which are combined with comments, information about units, pictures, and further structural information, like, for example, the information that the settings for the time step control need only be requested for transient problems. Using this list, `WIAS-MatConE` allows to create and edit the considered type of file within a GUI framework.

`WIAS-MatConE` provides a fast and flexible way to generate GUIs for prototypical software without having to deal with the details of GUI development.

WIAS-SHarP (contact: D. Hömberg, phone: +49 30/20372-491)

Based on pdelib, WIAS–SHarP (**S**urface **Har**dening **P**rogram) is a software for the simulation of electron and laser beam surface hardening. It contains a data bank with material parameters for 20 important steels as well as routines to describe the phase transition kinetics during one heat treatment cycle. Moreover, it allows for an easy implementation of different radiation flux profiles. In the new version, an adaptive grid is used. To facilitate its usage, a Java-based GUI has been developed.

For more information see http://www.wias-berlin.de/software/sharp.

WIAS-TeSCA (contact: R. Nürnberg, phone: +49 30/20372-570)

WIAS–TeSCA is a **T**wo- and thre**e**-dimensional **S**emi-**C**onductor **A**nalysis package. It serves to simulate numerically the charge carrier transport in semiconductor devices based upon the drift-diffusion model. This van Roosbroeck system is augmented by a vast variety of additional physical phenomena playing a role in the operation of specialized semiconductor devices, as, e.g., the influence of magnetic fields, optical radiation, temperature, or the kinetics of deep (trapped) impurities.

The strategy of WIAS–TeSCA for solving the resulting highly nonlinear system of partial differential equations is oriented towards the Lyapunov structure of the system that describes the currents of electrons and holes within the device. Thus, efficient numerical procedures, for both the stationary and the transient simulation, have been implemented, the spatial structure of which is a finite volume method. The underlying finite element discretization allows the simulation of arbitrarily shaped two-dimensional device structures.

WIAS–TeSCA has been successfully used in the research and development of semiconductor devices such as transistors, diodes, sensors, detectors, and lasers.

The semiconductor device simulation package WIAS–TeSCA operates in a UNIX environment and is available for a variety of configurations as, e.g., SUN, COMPAQ, but also for Linux PC.

For more information please see http://www.wias-berlin.de/software/tesca.

WIAS-QW (contact: U. Bandelow, phone: +49 30/20372-471)

WIAS–QW is a numerical code for the simulation of strained multi-quantum-well structures. Based upon multi-band kp models it allows to treat band mixing effects, confinement effects, crystal symmetry, and the influence of mechanical strain.

In particular, WIAS–QW calculates the

- subband dispersion
- eigenfunctions
- transition matrix elements
- miniband effects in multi-quantum-well structures

In dependence on the sheet carrier densities and the temperature, WIAS–QW calculates the

- optical response function
- gain spectrum
- radiative recombination rate
- carrier density distributions

Furthermore, the calculations can be done selfconsistently, comprising pure kp calculations, but also calculations that include the Hartree–Coulomb potential, obtained from Poisson's equation, as well as density-

dependent exchange-correlation potentials accounting for the bandgap-shift, which is one of the most prominent many-particle effects.

Please find further information under http://www.wias-berlin.de/software/qw.