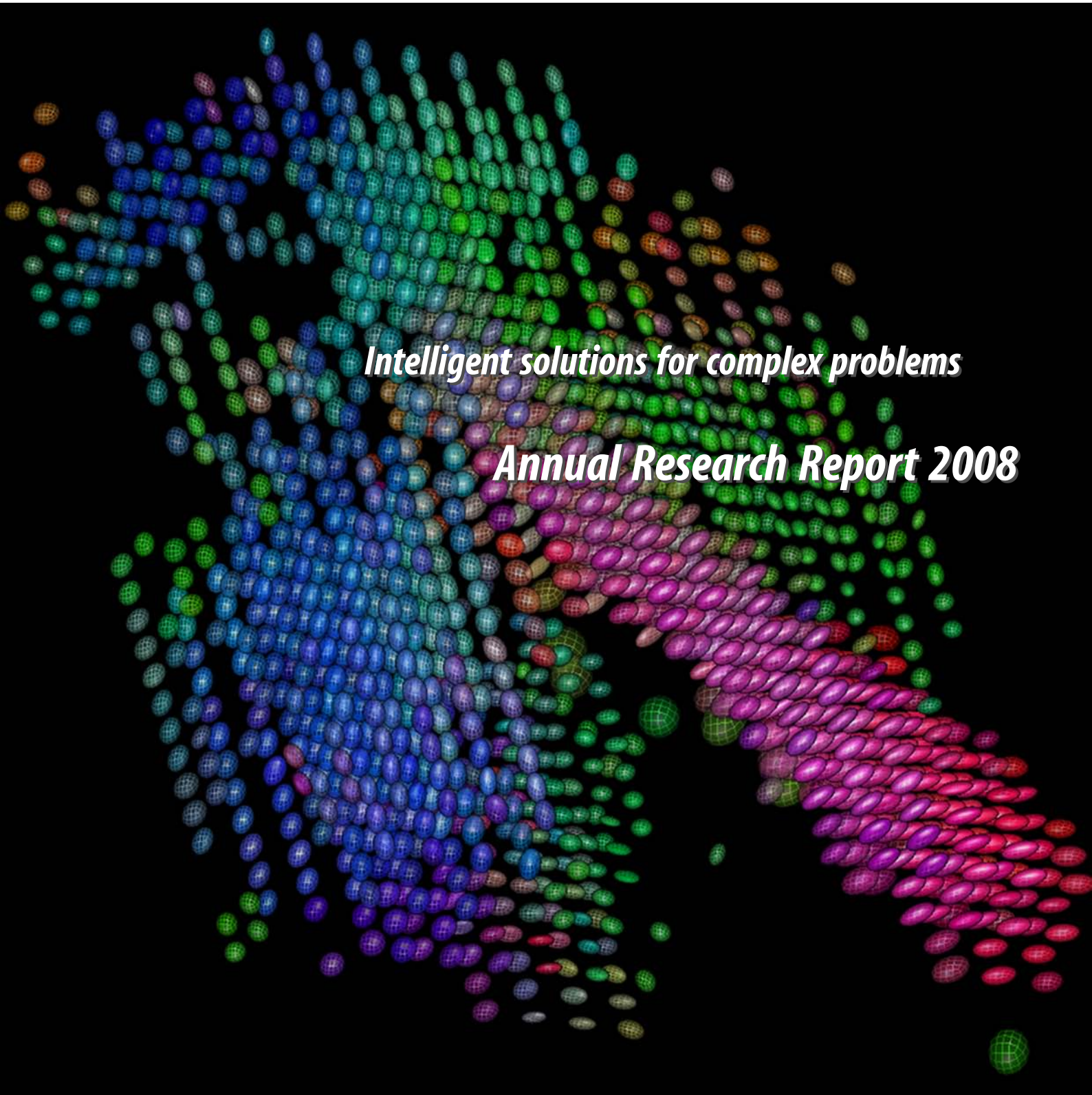
WIAS

Weierstrass Institute for Applied Analysis and Stochastics

Leibniz Gemeinschaft

Forschungsverbund Berlin e.V.



Intelligent solutions for complex problems

Annual Research Report 2008

Cover figure: Diffusion Tensor Imaging (DTI): Tensor field reconstruction from diffusion weighted imaging data.

Edited by Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
D – 10117 Berlin
Germany

ISSN 1437-7489
Berlin 2008

Fax: + 49 30 2044975
E-Mail: contact@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Prof. Dr. Jürgen Sprekels, Director

The Weierstrass Institute for Applied Analysis and Stochastics (WIAS, member of the Leibniz Association) presents its Annual Report 2008. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2008. 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.

The year 2008 was marked by continuing last year's successful work in the *Research Program 2007–2009*. WIAS further 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 further 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
- Flow and transport processes in continua
- Stochastics in science and economics
- Numerical methods of analysis and stochastics

Besides the international workshops organized by the institute, the increased number of invited lectures held by WIAS members at international meetings and research institutions, and the many renowned foreign visitors hosted by the institute last year, the positive development is best reflected by the largest acquisition of grants ever. After having crossed the "magic line" of two million euros in 2007 for the first time, the total grants acquired in 2008 exceeded 2.5 million euros, another substantial increase! More than thirty-five additional co-workers could be financed from these grants.

In addition to this, WIAS was in 2008 for the second time successful in the Excellence Competition of the Leibniz Association: Dr. Dorothee Knees and Dr. Christiane Kraus will jointly head from 2009 to 2011 the new Leibniz Group on "Modeling of Damage Processes". Besides the two group leaders, one postdoc and two doctoral students will be financed within this project. It is noteworthy that in this way for the first time ever a group at WIAS will be headed by female scientists. This fact witnesses the institute's continuing efforts to support female scientists.

Concerning refereed journal publications, 2008 brought a strong increase in comparison with 2007. In addition, four excellent monographs, which were edited by WIAS members, appeared in renowned scientific series of top-selling publishing companies. In addition to this, WIAS members made major contributions to a number of further monographs.

As special highlight of the year 2008, and as a convincing recognition that the research at WIAS is of great importance for the development of science and high technology, the prestigious "Innovation Prize Berlin-Brandenburg 2008" was in December awarded to WIAS as part of the KRIST*MAG*® consortium. In this consortium, which was financially supported by Technologiestiftung Berlin

(TSB) and EFRE, groups at the *Leibniz Institute of Crystal Growth (IKZ)* and at WIAS had joined forces with the industrial companies *Steremat Elektrowärme* and *Auteam* to develop a new technology for the growth of semiconductor crystals using so-called *traveling magnetic fields*.

The high rank of WIAS in the mathematical community was again witnessed by the fact that the year-long success story of "Transfer of knowledge via brains" through the institute's members continued also in 2008: Prof. Dr. Anton Bovier accepted a full professorship at the Universität Bonn. In addition to that, Dr. Christian Meyer first declined an offer for a junior professorship at the RWTH Aachen and then accepted the offer for a junior professorship at the Technische Universität Darmstadt. Since the institute's foundation in 1992, a total of 37 calls (including 17 to full professorships in Germany and nine to professorships abroad) have been received by WIAS members, a truly remarkable output of which we are proud.

Eight international workshops organized by WIAS 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, Prof. Jürgen Sprekels served as co-organizer of a conference at the Mathematisches Forschungsinstitut Oberwolfach (MFO). Also the guest program of WIAS was intensified in 2008 by hosting the group of winners of the Weierstrass Postdoctoral Fellowships (see page 145).

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 four leading members of WIAS, including the director and his deputy, hold special chairs funded by WIAS at the Berlin universities. Two further such appointments are under way, and we are hoping that by the end of 2009 six WIAS members will hold chairs funded by WIAS at the Berlin universities.

The highlight of cooperation with the mathematical institutions in Berlin was also in 2008 the joint operation of the DFG Research Center MATHEON "Mathematics for key technologies" located at the Technical University of Berlin. MATHEON is presently in its second period, which extends until May 2010. DFG funds exceeding 5.5 million euros per year continue to 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 member of MATHEON's Executive Board, his deputy is associated member of the Executive Board, PD Dr. Barbara Wagner is deputy chair of the MATHEON Council, and several members of WIAS serve as *Scientists in Charge* of mathematical fields or of application areas in the center. Besides, WIAS members participate in the management of 18 of its subprojects. In turn, in 2008 up to 17 scientific collaborators and several student assistants employed at WIAS were funded by MATHEON.

Another big success story for the mathematical community of Berlin is the "Berlin Mathematical School" (BMS), which had been won in the framework of the German "Competition for Excellence". The BMS, a graduate school for advanced mathematical studies, brings together the capacities of all mathematical institutions in Berlin to attract excellent doctoral students from all over the world. Also in this application, members of WIAS took part as principal investigators, and many members of WIAS serve in the BMS, teaching courses and supervising doctoral students.

Besides these major 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 Research Training Groups of the German Research Foundation (DFG). For example, the institute contributes considerably to the operation of the DFG Research Training Group "Analysis, Numerics, and Optimization of Multiphase Problems" at the Humboldt University of Berlin, and Prof. Anton Bovier served as the Speaker of the International DFG Research Training Group "Stochastic Models of Complex Processes", which combines groups from the Technical and the Humboldt University, WIAS, and the University of Potsdam, with groups from the University of Zurich and the ETH Zurich. Also, WIAS groups participate in the various DFG Collaborative Research Centers.

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. The recent achievements give evidence that this concept, in combination with hard, continuing work in scientific details, eventually leads to success.

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 February 2009

J. Sprekels

Scientific Advisory Board

Chairman:

Prof. Dr. F. R. Götze
Universität Bielefeld, Fakultät für Mathematik
Postfach 10 01 31, 33501 Bielefeld

Vice Chairman:

Prof. DI. Dr. K. Kunisch
Karl-Franzens-Universität Graz
Institut für Mathematik und Wissenschaftliches Rechnen
Heinrichstraße 36, 8010 Graz, Austria

Prof. Dr. A. Gilg
Siemens AG, CTPP2
Otto-Hahn-Ring 6, 81739 München

Prof. Dr. W. Th. F. den Hollander
Leiden University, Mathematical Institute
P.O. Box 9512, 2300 RA Leiden, The Netherlands

Prof. Dr. B. Niethammer
University of Oxford, Mathematical Institute
24–29 St Giles', Oxford OX1 3LB, UK

Prof. Dr. F. Otto
Universität Bonn, Institut für Angewandte Mathematik
Wegelerstraße 10, 53115 Bonn

Dr. A. Schuppert
Bayer Technology Services
Director Process Technology M & T CS
Bayer AG, Building K 9, 51368 Leverkusen

Prof. Dr. Ch. Schwab
ETH Zürich, Seminar for Applied Mathematics
ETH Zentrum, HG G58.1
Rämistrasse 101, 8092 Zurich, Switzerland

Dr. U. Thiel
Vice President Cray Europe
Waldhofer Straße 102, 69123 Heidelberg

1 WIAS in 2008

- 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 optimize the common efforts of the institute's scientific staff.

WIAS is dedicated to education on all levels, ranging from the teaching of numerous classes at the Berlin universities to the supervision of theses and of two trainees in the profession of a "mathematical technical software developer".

1.2 Structure and Scientific Organization

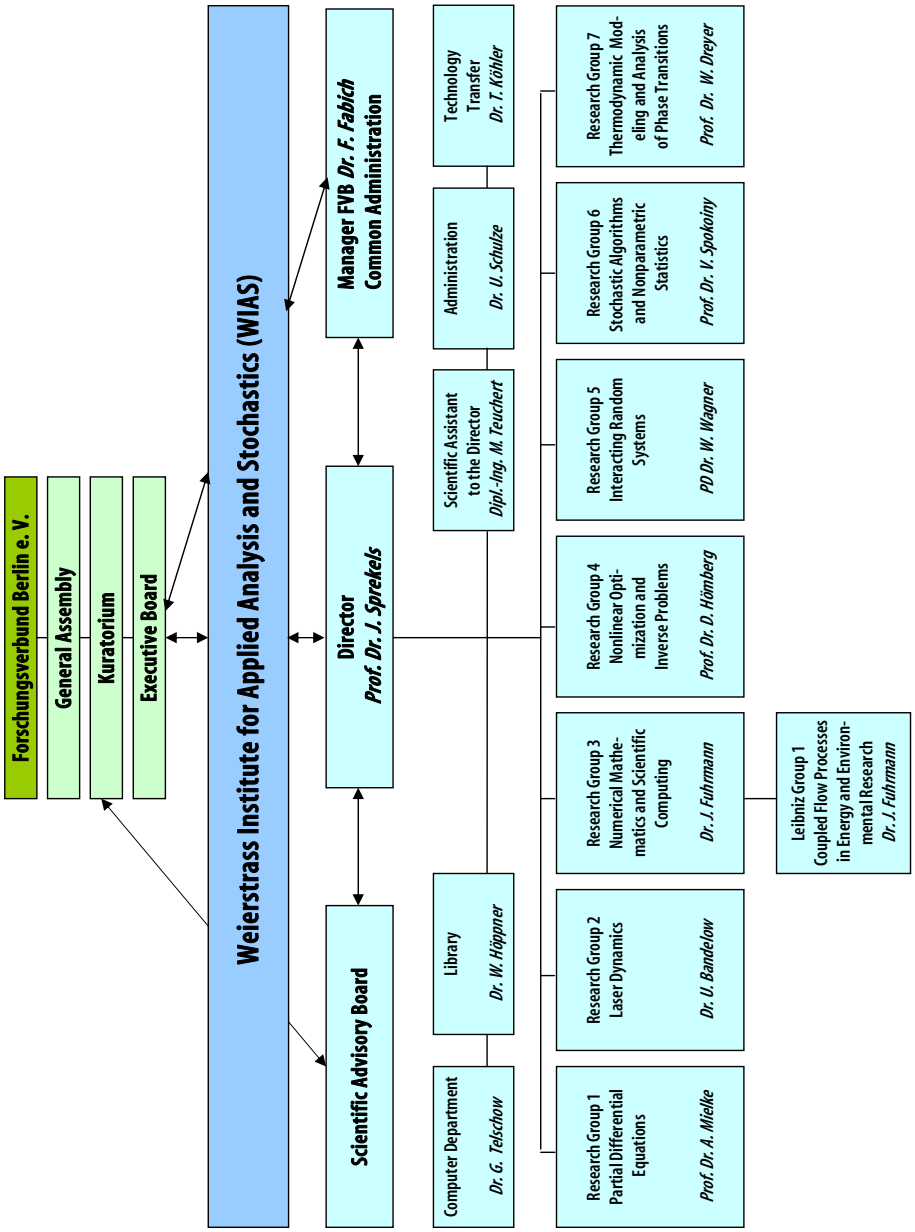
1.2.1 Structure

To fulfill its mission, WIAS was in 2008 structured in departments for technical services, the seven scientific research groups, and one Leibniz group[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
LG 1. Coupled Flow Processes in Energy and Environmental Research

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

The following organization chart gives an overview of the organizational structure of WIAS in 2008:



1.2.2 Main Fields of Research

The research at WIAS focused in 2008 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**
- **Flow and transport processes in continua**
- **Stochastics in science and economics**
- **Numerical methods of analysis and stochastics**

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

- **Optical technologies** (in particular, optical fibers, lasers, and diffractive structures)
- **Fuel cells** (direct methanol fuel cells),
- **Crystal growth**

1.2.3 Contributions of the Research Groups of WIAS

The seven research groups and the Leibniz group form the institute's basis to fully bring to bear and develop scope and depth of its expertise. The mathematical problems studied by the 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 and Leibniz groups contributed in 2008 in the interdisciplinary solution process described above.

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

In the following, we list special research topics that were addressed in 2008 within the general framework of the main fields. The research and Leibniz groups that contributed to the respective studies are indicated in brackets.

1. Nano- and optoelectronics

- Microelectronic devices (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 and their consistent coupling to macroscopic models (in RG 1)
- Laser structures (in RG 2)
- Fiber optics (modeling of optical fields in nonlinear dispersive optical media; in 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 (in RG 1 and RG 7)
- Modeling of damage and crack propagation in elastic materials (in RG 1)
- 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)
- Formation and evolution of microstructures in elastoplasticity (in RG 1 and RG 7)
- Stochastic modeling of phase transitions (in RG 5)
- Growth of semiconductor bulk single crystals (silicon carbide, silicon, gallium arsenide; in RG 7)

4. Flow and transport processes in continua

- Treatment of Navier–Stokes equations (in RG 3, RG 7, and LG 1)
- Flow and mass exchange in porous media (water and materials transport in soils and in porous rocks, two-phase flows; in RG 3 and LG 1)
- Modeling of fuel cells (in RG 3)
- Modeling of nanostructures of thin films on crystalline surfaces (in RG 7)

5. 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)

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 (see page 159)

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 very successful in 2008, having raised a total of 2.6 million euros, from which additional 34 researchers (+ 4 outside WIAS; Dec. 31, 2008) have been financed. Particularly important is the fact that the funds raised in industrial collaborations could be increased to 0.5 million euros. In total, 27.3 per cent of the total budget of WIAS in 2008 and 37.9 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 was the joint operation of the DFG Research Center MATHEON "Mathematics for key technologies". Following a very successful evaluation by an international panel of referees in January 2006, MATHEON was granted a second funding period until 2010. Annually, DFG funds exceeding 5.5 million euros flow into Berlin for MATHEON. In 2008, WIAS dedicated considerable financial and personal resources to the Center: Its director was a member of MATHEON's Executive Board, both his deputies were "Scientists in Charge" of mathematical fields in the Center, B. Wagner (RG 7) was elected Deputy Chairperson of its Council, and members of WIAS participate in the management of 18 of its subprojects. In turn, in 2008 up to 17 scientific collaborators and several student assistants at WIAS were funded by MATHEON.

1.3.2 Graduate School *Berlin Mathematical School (BMS)*

Berlin's mathematicians won this graduate school, which is run by the three major Berlin universities, within the framework of the German Initiative for Excellence in 2006 in a joint effort. Funds exceeding one million euros per year for the BMS, which started operations in the fall of 2006, strengthen for five years the efforts of the mathematical institutions of Berlin to attract excellent young Ph.D. students to the city. Among the principal investigators of this successful initiative have been both Deputy Directors of WIAS, Profs. A. Bovier (RG 5) and A. Mielke (RG 1). Many further members of WIAS contributed to the operations of the BMS.

1.3.3 International Research Training Group 1339 *Stochastic Models of Complex Processes* of the DFG

This international graduate college, which is operated jointly with ETH Zürich and University of Zurich, Switzerland, is another big success of the activities of Berlin's mathematicians. The graduate college, whose first funding period runs from July 2006 to December 2011, is located at the Technical University of Berlin; its Coordinator is Prof. A. Bovier, who was until October 2008 the second Deputy Director of WIAS.

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

1.3.4 DFG Research Training Group GRK 1128 *Analysis, Numerics, and Optimization of Multiphase Problems*

In the Research Training Group GRK 1128 at the Humboldt University of 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. WIAS members are presently supervising the theses of seven graduates.

1.3.5 DFG Research Unit 797 *Analysis and Computation of Microstructure in Finite Plasticity*

WIAS participates in this research unit in the sub-project "Regularizations and relaxations of time-continuous problems in plasticity" (RG 1; first funding period: until August 2010).

1.3.6 DFG Collaborative Research Center (SFB) 649 *Economic Risk*

This research project, which has been funded by the DFG since 2005, focuses on studying economic risk. The Weierstrass Institute participates in two sub-projects: "Structural adaptive data analysis" and "Calibration and pricing errors in risk management" (both RG 6). The SFB has been positively evaluated in September 2008 and prolonged for the next period until the end of 2012.

1.3.7 DFG Collaborative Research Center (SFB) 787 *Semiconductor Nanophotonics: Materials, Models, Devices*

This Collaborative Research Center began its work on January 1, 2008 (first funding period: until December 2011). WIAS participates in the sub-projects "Multi-dimensional modeling and simulation of VCSELs" (RG 1 and RG 2) and "Effective models, simulation and analysis of the dynamics in quantum-dot devices" (RG 2 and RG 7).

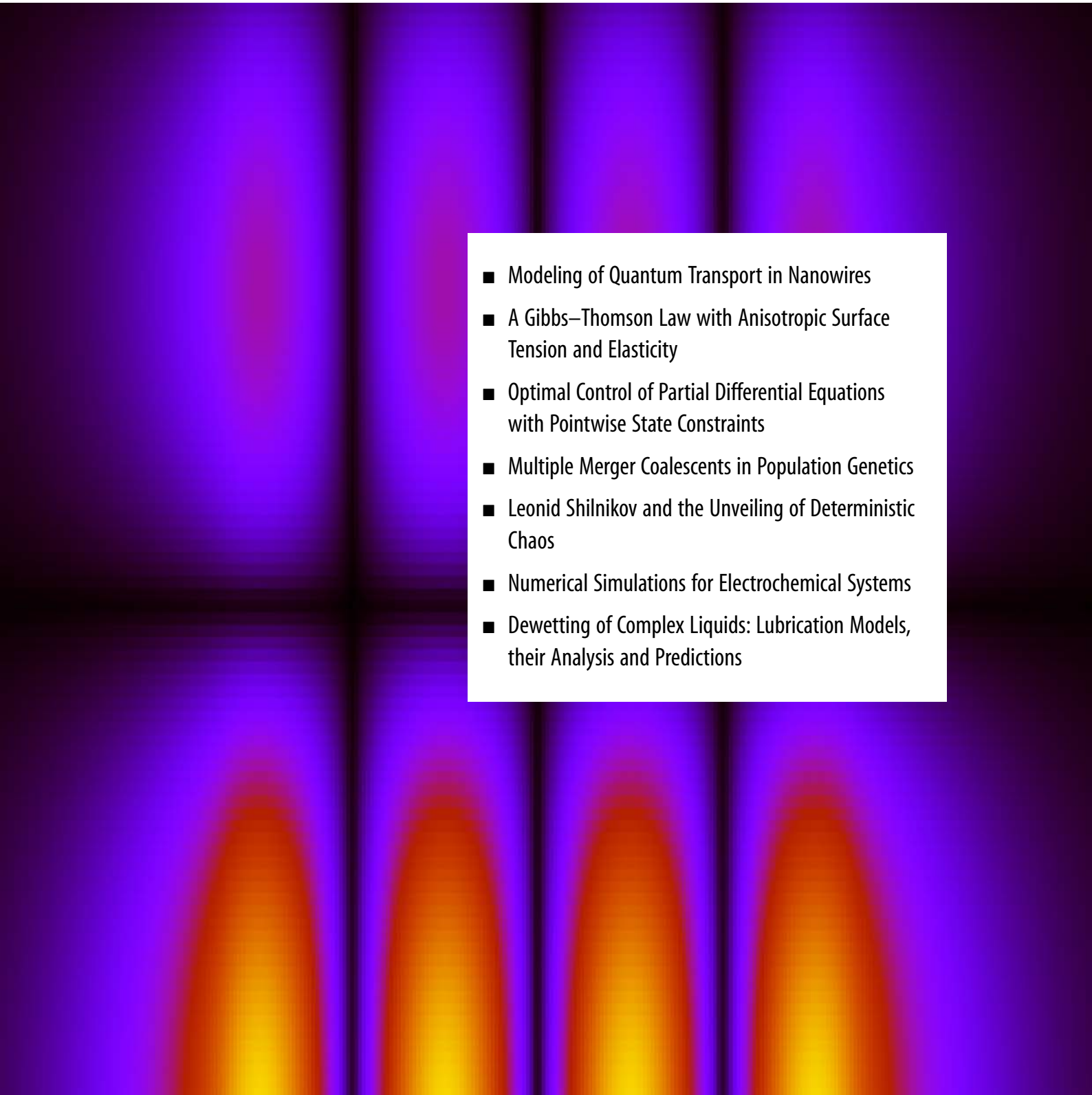
1.3.8 KRISTMAG®

This research project, which was funded from July 2005 to July 2008 by the "Zukunftsfonds" of the state of Berlin and headed by the Institute of Crystal Growth in Berlin-Adlershof, where WIAS cooperated with several industrial companies and other research institutions to develop a new technique for the crystal growth from a melt under the impact of traveling magnetic fields, has been bestowed in December the Innovation Prize Berlin/Brandenburg 2008.

1.3.9 BMBF Project *Numerical Simulation for Direct Methanol Micro Fuel Cells*

This research project, which started operations in 2005 and ran until June 2008, was funded by the German Ministry of Education and Research in the framework of the funding program "Networks for Basic Research in Renewable Energies and Energy Efficiency". It was part of an interdisciplinary joint project for the experimental investigation, modeling, and numerical simulation of direct methanol micro fuel cells, which was coordinated by the acting head of RG 3, Dr. J. Fuhrmann.

2 Scientific Highlights



- Modeling of Quantum Transport in Nanowires
- A Gibbs–Thomson Law with Anisotropic Surface Tension and Elasticity
- Optimal Control of Partial Differential Equations with Pointwise State Constraints
- Multiple Merger Coalescents in Population Genetics
- Leonid Shilnikov and the Unveiling of Deterministic Chaos
- Numerical Simulations for Electrochemical Systems
- Dewetting of Complex Liquids: Lubrication Models, their Analysis and Predictions

2.1 Modeling of Quantum Transport in Nanowires

Hagen Neidhardt and Paul Nicolae Racec

The ongoing requirement for scaling down semiconductor devices has lead to the development of various transistor architectures at low dimensions and with improved characteristics compared to the metal-oxide-semiconductor field-effect transistor in bulk silicon. The International Technology Roadmap for Semiconductors has established the nanowire field-effect transistor as a promising technology candidate for applications in logic. Very recently [1], Samsung Electronics Co. has fabricated a silicon nanowire field-effect transistor with nanowire of radius $R = 4$ nm and gate length $L = 15$ nm by a technological process that can be realized with today's industrial equipment.

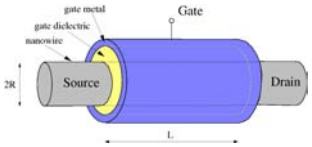


Fig. 1: *Sketch of a nanowire transistor*

Nanowire transistors are based on a cylindrical geometry; see Figure 1. The main current flows through the central wire from one end, called *source contact*, to the other end, called *drain contact*. The gate is wrapped around the wire. Applying suitable voltages to the gate, the current flowing from source to drain can be controlled.

Nowadays, semiconductor devices at nanoscale dimensions have reached the quantum transport regime with its characteristic effects: for instance, the tunneling of electrons through narrow potential barriers and the quantization of energy. The most intriguing aspect of quantum transport is the formation of resonances that allow for the design of new electrical properties of the semiconductor devices.

The research done in the last years has led to nanowire-based semiconductor devices with progressively increased structural complexity like nanowire resonant tunneling diodes [2], qubits [3], or lasers [4]. In developing and optimizing such ultra-small devices, the simulation gains more and more importance [5], because of the very time-consuming and expensive production processes. We present here a new approach allowing the calculation of the key features of nanowire transistors.

Scattering states and tunneling coefficients

The goal of modeling the nanowire transistor is to calculate the current for given source, drain, and gate voltages. Since the dimensions are very small, a quantum description is required for which the main ingredients are the Schrödinger operator and the wave function $\psi(r, \theta, z)$. It is important to note that one has to treat the nanowire as an *open quantum system*, because current flows or tunnels from source to drain. The key quantity describing the tunneling is the so-called *total tunneling coefficient* $T(E)$. The total current going from source to drain is then obtained via the so-called *Landauer–Büttiker formalism* in which $T(E)$ enters [6].

To determine the total tunneling coefficient $T(E)$, one has to solve the scattering problem for the three-dimensional Schrödinger equation for the whole nanowire, where the potential $V(r, \theta, z)$ encodes the different material properties. The azimuthal symmetry suggests to use cylindrical coordinates with the z-axis along the nanowire. Thus, the θ-dependence is taken into account by an

infinite number of Schrödinger equations

$$\underbrace{-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{m^2}{r^2}\right)}_{\text{radial Hamiltonian}}\psi^{(m)}(r,z)+\underbrace{\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2}+V(r,z)\right)}_{\text{channel Hamiltonian}}\psi^{(m)}(r,z)=E\psi^{(m)}(r,z), \qquad (1)$$

defined on the unbounded domain $r \in [0, R], z \in (-\infty, \infty)$, cf. Figure 2, labeled by the so-called *magnetic quantum number* $m = 0, \pm 1, \pm 2, \ldots$. For each m, one has to solve the scattering problem. In this way, every magnetic quantum number m defines a *two-dimensional (2D) scattering problem*. How many of these problems have to be solved depends on the specific physical quantity that has to be computed. The radial Hamiltonian, which is supplemented by Dirichlet boundary conditions due to the confinement of the electrons inside the nanowire, defines the so-called *channels* with the energy $E_{\perp n}^{(m)}$ and channel eigenfunctions $\phi_n^{(m)}(r)$, $n = 1, 2, \ldots$, $m = 0, \pm 1, \pm 2, \ldots$. It is worth to mention here that the channel n can be uniquely identified by the number of maxima and the number of zeros of the channel eigenfunction $\phi_n^{(m)}(r)$. In particular, for $m \neq 0$, $\phi_n^{(m)}(r)$ vanishes at the cylinder axis $r = 0$. These properties can be used as a "fingerprint" of the channel n, which helps to identify channels in experiments or simulations. The interaction between channels is described by the coupling matrix elements

$$V_{nn'}^{(m)}(z) := \int_0^R \phi_n^{(m)}(r) V(r,z) \phi_{n'}^{(m)}(r)\, r\, dr.$$

The nanowire design leads to potentials V that depend nontrivially on (r, z) in the scattering region $-d_z \leq z \leq d_z$ and are called *scattering potentials* $V(r, z)$, while they are constant outside, namely V_1 in the source and V_2 in the drain; see Figure 2. An electron coming from the source is scattered by this potential. During this process, the electron with energy E can either be reflected by the potential and return to the source, or it can reach the drain, passing the zone $[-d_z, d_z]$. In both cases, the electron has to move in one of the channels. However, by the energy conservation law, not every channel is allowed, but only the open ones. For an electron of energy E, the channel $\phi_n^{(m)}$ is called *open* in the source or in the drain if $E \geq E_{\perp n}^{(m)} + V_1$ or $E \geq E_{\perp n}^{(m)} + V_2$, respectively. Otherwise, a channel is called *closed*.

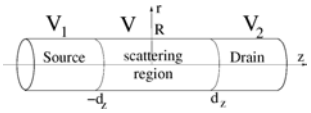


Fig. 2: *Geometry of the 2D scattering problem*

Consider an electron with energy E coming from the source. If for this energy there is an open channel n in the source and an open channel n' in the drain, then the electron can propagate from the source to the drain. The probability for this scattering process is called the *tunneling coefficient*, which is denoted by $T_{nn'}(E)$ [6, 8]. Of course, the tunneling coefficient is zero if the channel n' in the drain is closed. The total tunneling coefficient $T(E)$ is defined as a sum over all tunneling coefficients between possible channels n and n'.

The total tunneling coefficient is technologically important, since it determines the current going through the nanowire. These coefficients are very efficiently computed by the so-called *R-matrix formalism* [6, 7, 8]. The main idea is to find an appropriate basis of functions for the wave functions restricted to the scattering region. This basis is provided by the Wigner–Eisenbud functions, which are solutions of the Schrödinger equation in the scattering region satisfying appropriate boundary conditions. In such a way, one solves only once an eigenvalue problem in the scattering region, and the solutions of equation (1) are found for every energy E by low-dimensional matrix

multiplication. This numerical implementation does not need a discretization of the energy axis, which would increase enormously the computation costs in order to resolve sharp resonances and the associated peaks and dips in the tunneling coefficient.

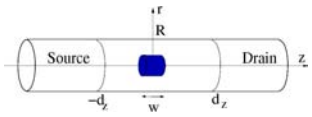


Fig. 3: *Sketch of a quantum dot embedded into the nanowire*

Since the resonances dominate the electrical properties of the device, the precise description of the peaks and dips in $T(E)$ is essential for the improvement and design of semiconductor devices. Hence, the method developed in [8] provides a first simple tool to analyze in detail the resonances in nanowire heterostructures. Below, we show the power of the method by treating two model systems.

Quantum dot embedded inside the nanowire

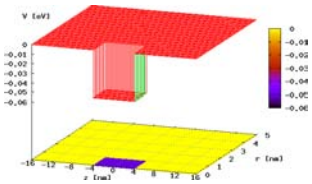


Fig. 4: *Quantum-well potential of depth* $W_b = -0.05$ *eV, width* $w =$ *8 nm, and* $R' = 1$ *nm*

In the following, we study a cylindrical dot embedded into the nanocylinder, but its radius R' is smaller than the cylinder radius R. Therefore, the dot is surrounded by the host material; see Figure 3. Depending on the potential difference W_b between the dot material and the host material, the dot can be repulsive, yielding a quantum barrier, or attractive, yielding a quantum well. The parameters are $R = 5$ nm, the effective mass $\mu = 0.19\, m_0$ (corresponding to the transverse mass in silicon), $d_z = 16$ nm, and the total number of channels (open and closed) $N = 8$.

We consider the case that the scattering potential is attractive; see Figure 4. The diagonal coupling matrix elements $V_{nn}(z)$ act for every channel n as an effective one-dimensional attractive potential, which yields the existence of at least one bound state below the channel energy $E_{\perp n}^{(m)}$. By mixing the channels, we obtain resonances, which can be seen as dips in the tunneling coefficient in Figure 5 for different depths of the quantum well.

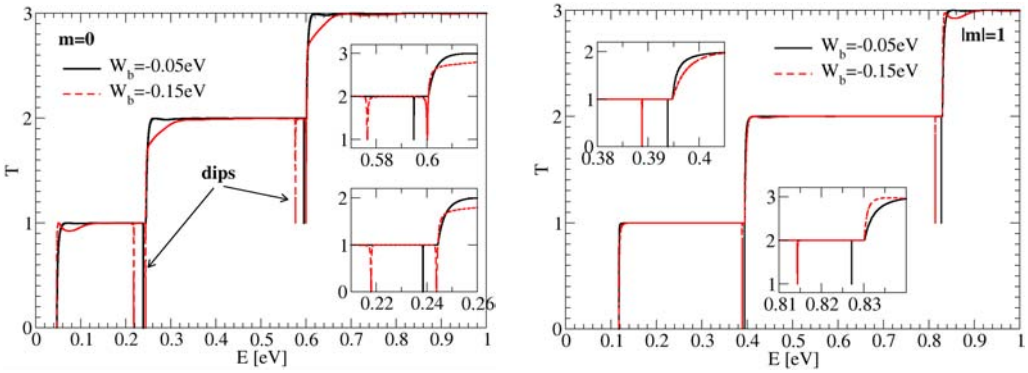
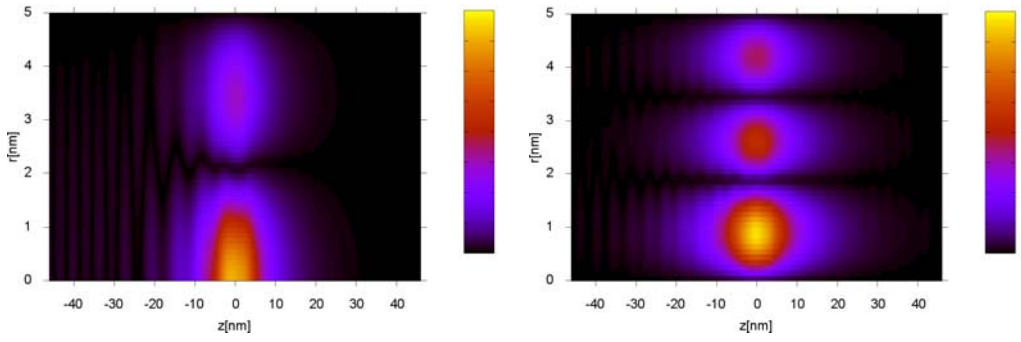


Fig. 5: *Total tunneling coefficient for the scattering potential in Figure 4*

Further insight about these resonances can be gained looking at the *localization probability density* $|\psi_n^{(m)}(E, r, z)|^2$ obtained from our numerical implementation based on the R-matrix formalism [8]. In Figure 6, we represent the localization probability density of an electron that is incident from the source and has a total energy corresponding to the dips in Figure 5. The localization probability has a pronounced peak around the quantum well and decreases exponentially to the left and to the right. In order to establish the origin of this resonance, we look at the "fingerprint" of the channel. Figure 6a shows that the scattering wave is incident on the first channel, which has no zeros and one maximum in the r-direction, but inside the scattering region has a zero and two maxima

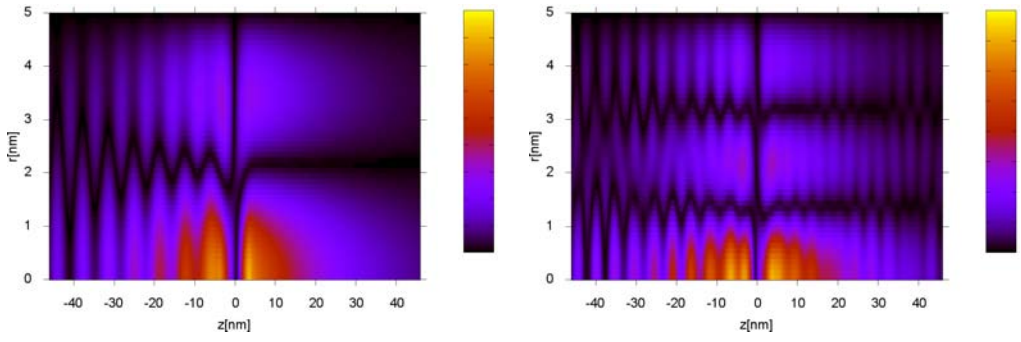
in the r-direction, which is characteristic for the second channel. One gets similar pictures for all m values. In Figure 6b for the case $|m| = 1$, the scattering wave is incident on the second channel and should have one zero and two maxima in the r-direction, but inside the scattering region, it has two zeros and three maxima in the r-direction, which is typical for the third channel. Hence, the method allowed us to explain in detail the resonance mechanism via closed channels.



(a) $m = 0$, $E = 0.238$ eV, $n = 1$ (b) $|m| = 1$, $E = 0.827$ eV, $n = 2$

Fig. 6: *Localization probability density for the dips in Figure 5 and for $W_b = -0.05$ eV*

Increasing the strength of the attractive potential to $W_b = -0.15$ eV, one can see more dips in the tunneling coefficient in Figure 5. It is interesting to note that there are two dips in the first and second plateau for $m = 0$, while for $|m| = 1$, there is only one dip in every plateau. In the case of $m \neq 0$, the transversal modes $\phi_n^{(m)}(r)$ are zero on the cylinder axis, so that the effective potential $V_{nn}(z)$ for every channel is weakened. To confirm that the dips correspond to the higher-order bound states of closed channels, we plot in Figure 7 the localization probability density of the scattering states at the energies corresponding to the second dip in every plateau for $m = 0$. One can see that the scattering states have an additional zero in the z-direction at $z = 0$. The structure of zeros in the r-direction shows that their origins are eigenstates of the second and third channel, respectively, which are closed channels.



(a) $m = 0$, $E = 0.243$ eV, $n = 1$ (b) $m = 0$, $E = 0.600$ eV, $n = 2$

Fig. 7: *Localization probability density for the dips in Figure 5 for $W_b = -0.15$ eV*

Double-barrier heterostructure along the nanowire

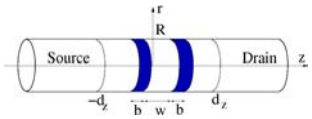


Fig. 8: *Sketch of a double-barrier heterostructure along the nanowire*

Figure 8 shows a sketch of a double-barrier heterostructure along the nanowire. In Figure 9, the corresponding scattering potential $V(r,z)$ is represented. Further parameters are as in the previous case. In contrast to the first example, the potential is independent of r, and resonances are not a result of interacting channels, but they appear between the barriers. The physical interpretation of these resonances is that the electron is reflected or transmitted through the first barrier, reaches the second barrier, where it is again reflected or transmitted; the reflected part reaches now the first barrier, where it is again reflected or transmitted and so on. If all these forward and backward reflections between the barriers are coherent, then a resonance appears.

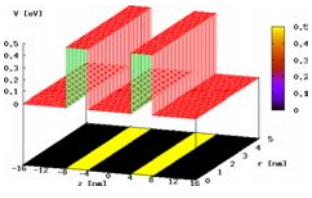


Fig. 9: *Double-barrier potential with $V_b = 0.5$ eV, $b = 4$ nm, and $w = 8$ nm*

The total tunneling coefficient $T(E)$ for $m = 0$ and $|m| = 1$ is plotted in Figure 10 in linear scale. One can observe a series of sharp peaks, with different positions for different m-values due to the dependence on m of the transversal energy channels $E_{\perp,n}^{(m)}$, represented by vertical dashed lines. One can also observe that the total tunneling coefficient can reach values higher than 1 if there are several open channels. These peaks differ substantially from the resonances presented in the previous section and are given by the resonances between the barriers [8]. The "fingerprint" of the wave function in the r-direction gives now information about the incident open channel.

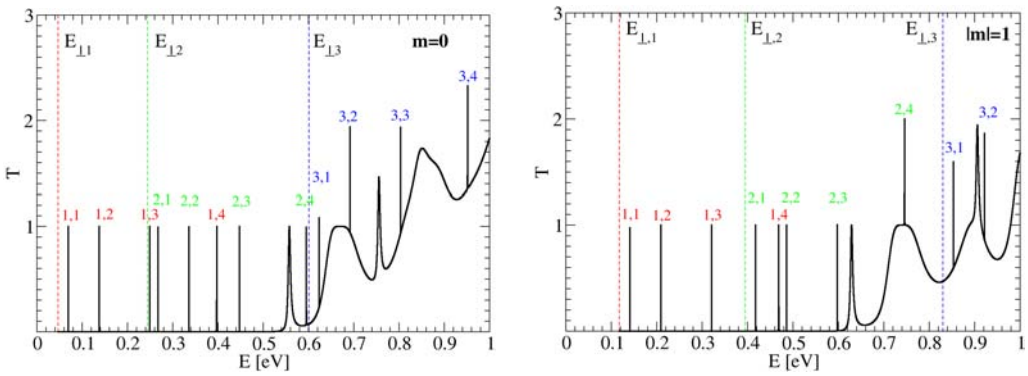


Fig. 10: *Transmission probability for a double barrier along the nanowire. Left: $m = 0$, right: $|m| = 1$*

In such a way, our method enables us to label the peaks in the tunneling coefficient by a pair of numbers (n,i), where n describes the incident channel, and i labels the resonances between the barriers; in our case, there are four. Knowing the provenience of the resonances, one can use them selectively for designing specific electrical characteristics of the device. The localization probability densities, corresponding to the transmission peaks, are represented in Table 1 for $m = 0$. One can see that the wave functions are localized between the barriers, so they indeed correspond to resonances between barriers and not to bound states of closed channels. This provides a picture of the orbitals of the "artificial atom", which represents this quantum structure.

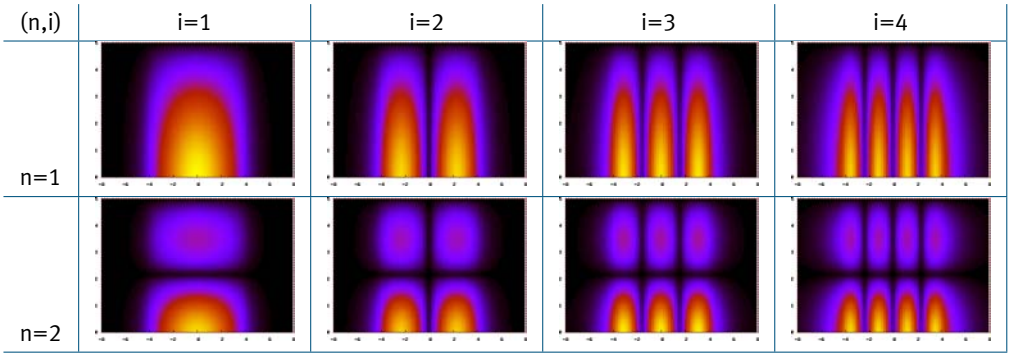


Table 1: *Localization probability density for resonant energies for* $m = 0$. *The axis of abscissae is* $z \in [-8, 8]$ *nm and the axis of ordinates is* $r \in [0, 5]$ *nm for all plots*

References

[1] K.H. Cho, K.H. Yeo, Y.Y. Yeoh, S.D. Suk, M. Li, J.M. Lee, M.-S. Kim, D.-W. Kim, D. Park, B.H. Hong, Y.C. Jung, S.W. Hwang, *Experimental evidence of ballistic transport in cylindrical gate-all-around twin silicon nanowire metal-oxide-semiconductor field-effect transistors*, Appl. Phys. Lett., **92** (2008), pp. 052102/1–052102/3.

[2] J. Wensorra, K.M. Indlekofer, M.I. Lepsa, A. Forster, H. Lüth, *Resonant tunneling in nanocolumns improved by quantum collimation*, Nano Lett., **5** (2005), pp. 2470–2475.

[3] Y. Hu, H.O.H. Churchill, D.J. Reilly, J. Xiang, C.M. Lieber, C.M. Marcus, *A Ge/Si heterostructure nanowire-based double quantum dot with integrated charge sensor*, Nature Nanotechnol., **2** (2007), pp. 622–625.

[4] F. Qian, Y. Li, S.G. Caronak, H.-G. Park, Y. Dong, Y. Ding, Z.L. Wang, C.M. Lieber, *Multi-quantum-well nanowire heterostructures for wavelength-controlled lasers*, Nature Mater., **7** (2008), pp. 701–706.

[5] D. Vasileska, D. Mamaluy, H.R. Khan, K. Ravela, S.M. Goodnick, *Semiconductor device modeling*, J. Comput. Theor. Nanosci., **5** (2008), pp. 999–1030.

[6] G.A. Nemnes, U. Wulf, P.N. Racec, *Non-linear I-V characteristics of nano-transistors in the Landauer–Büttiker formalism*, J. Appl. Phys., **98** (2005), pp. 084308/1–084308/8.

[7] J. Behrndt, H. Neidhardt, E.R. Racec, P.N. Racec, U. Wulf, *On Eisenbud's and Wigner's R-matrix: A general approach*, J. Differ. Equations, **244** (2008), pp. 2545–2577.

[8] P.N. Racec, E.R. Racec, H. Neidhardt, *Evanescent channels and scattering in cylindrical nanowire heterostructures*, WIAS Preprint no. 1376, 2008.

2.2 A Gibbs–Thomson Law with Anisotropic Surface Tension and Elasticity

Christiane Kraus

The "technological revolution" in the last 20 years is generating an ongoing miniaturization in the area of microelectronics caused by an increasing requirement for mobile devices like cell phones or laptops and multimedia systems. The demands on strength and lifetime of the materials used is considerably rising, while the structural size is continuously being reduced. Additionally, as a consequence of the technological trends, there is a huge amount of electronic waste containing hazardous substances, such as cadmium, mercury, and lead, which create threats to human health and the environment. For instance, the *annual amount of electronic waste in Germany alone exceeds more than four times the volume of the 140 m high CHEOPS pyramid in Egypt* (Source: BUND). The total failure of electronic devices often results from microcracks in solder joints.

Figure 1 illustrates the typical morphology in the interior of solder materials, which are used to join a microchip to a copper plate. It shows phase separation processes of a binary alloy consisting of tin and lead at 125°C.

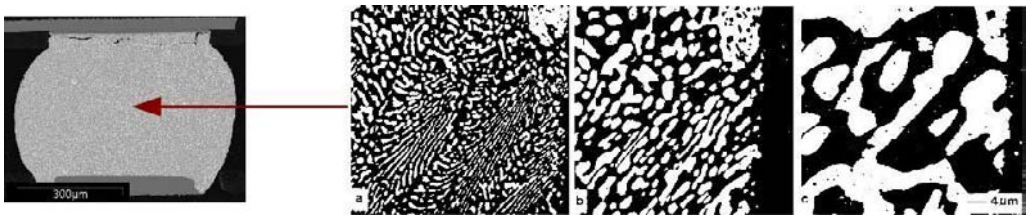


Fig. 1: *Left: Solder ball. Right: Microstructural coarsening in eutectic Sn-Pb a) directly after solidification, b) after three hours, and c) after 300 hours [4]*

The first stage of phase separation, the so-called *spinodal decomposition*, occurs on very short time and on very short spatial scales. A fine microstructure consisting of the original materials arises, since the system tries to minimize the chemical free energy. Then, coarsening phenomena, known as *Ostwald ripening*, take place. Larger particles grow, while smaller shrink, and particles coalesce. This process is mainly driven by the reduction of the surface energy.

During the separation process, one material starts to form precipitates within the other material, the matrix. The resulting "composite" can be regarded as a "particle reinforced material" in which the stiffer material acts as a reinforcement. Unfortunately, mechanical failure, such as cracks, can arise at the phase boundary due to thermal mismatching; cf. Figure 2.

Phase separation and coarsening processes are also observed phenomena in many other fields, including hydrodynamics, biology, chemistry, and material sciences. Such microstructural processes take place to reduce the total free energy, which may include the bulk chemical free energy, the interfacial energy, and the elastic strain energy.

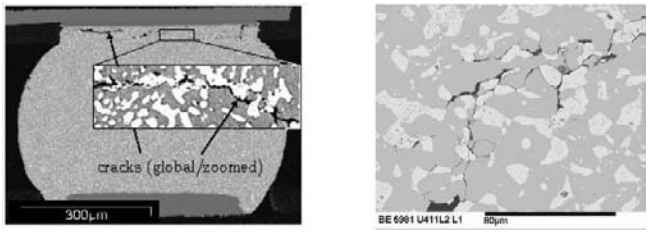


Fig. 2: *Crack initiation and propagation along the phase boundary [2]*

The knowledge of the mechanisms inducing phase separation and coarsening phenomena is of great importance for technological applications. A uniform distribution of the original materials is aimed to guarantee evenly distributed material properties of the sample. For instance, mechanical properties, such as the strength and the stability of the material, depend on how finely regions of the original materials are mixed. The control of aging and therefore of the lifetime of materials relies on the ability to understand phase separation and coarsening processes. This shows the importance of developing reliable mathematical models to describe such effects.

In the past few years, two different types of mathematical models have been primarily adopted: the *sharp interface* model and the *diffuse phase field* model. The conventional approach is the *sharp interface* model. Interfaces separating the coexisting phases or structural domains are modeled as hypersurfaces at which certain quantities suffer jump conditions. Local quantities at the interface, such as the chemical potential or the velocity, are then determined from the boundary conditions or are calculated from the driving force for interfacial motion and the interfacial mobility. This involves the explicit tracking of the interface and becomes often numerically impractical for complicated microstructures. Because of these disadvantages, the phase field approach has emerged as a powerful method during the last twenty years. It was introduced by Van der Waals more than a century ago, and in the context of phase separation in alloys, by Cahn–Hilliard in the nineteen sixties. The *diffuse phase field* model describes the interface between different phases as a small transition region, where an order parameter, representing the phases, changes its state smoothly. The microstructural evolution is modeled by a system of partial differential equations. Classical equations, in the context of phase separation and coarsening, are the Cahn–Hilliard, Cahn–Larché, and Allen–Cahn systems. The phase field model contains the corresponding sharp interface description as a particular limit. However, the rigorous derivation of the connection between these two kinds of models is often involved, and generalized formulations for the limit process are necessary to get convergence of diffuse phase field quantities in the sharp limit; cf. [5].

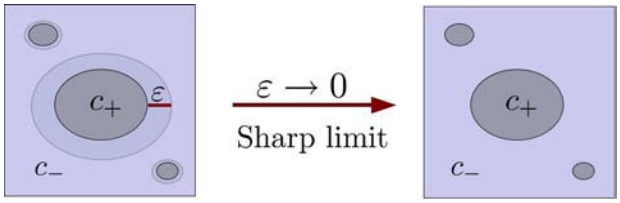


Fig. 3: *Left: Phase field model. Right: Corresponding sharp interface model*

In this article, we introduce a phase field model and determine the corresponding sharp interface limit. From the phase field approach, we establish a Gibbs–Thomson law in the sharp limit, which connects local quantities at the phase boundary to a function in the bulk, such as the chemical potential. The Gibbs–Thomson law states the system is in local equilibrium.

We consider in particular phase field models, which are capable to model *anisotropic surface tension* and *elastic effects* because models without these dependences have certain real-life limitations: they would only model cases where the particles are round and the larger ones always grow at the cost of smaller ones. This is sufficient for Ni-Al-Si alloys, see Figure 4, left, but not for SN-Pb and Al-Si alloys. For these alloys, the phase boundary grows along some direction, as pictured in Figure 1 and Figure 4, right. One reason for this behavior are elastic effects, which can result from the fact that the materials used like to take different volumes. This is, for instance, the case if the materials have different lattice structures. Another reason can be that one material is stiffer than the other.

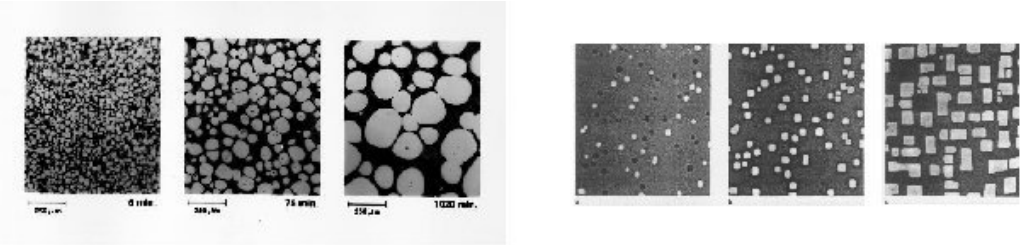


Fig. 4: *Left: Phase separation processes of Ni-Al-Si. Right: Phase separation processes of Ni-Al [5]*

The phase field model

Within the model, we restrict ourselves to binary alloys systems. The concentration c_0 of the system is fixed so that the concentrations of the two materials c_- and c_+ satisfy the condition $c_- + c_+ = c_0$ everywhere. This implies that the concentration difference $c = c_+ - c_-$ suffices to specify the distribution of the materials. Domains where $\{c \approx c_+\}$ or $\{c \approx c_-\}$ represent the two coexisting materials/phases are separated by a *diffuse* interface. The phase field model is based on a free energy functional.

Energy functional. The explicit structure of the free energy for binary alloys was deduced in [1] from the atomic level by means of pair potentials of Lennard–Jones type and the Embedded-Atom Method (EAM), a recently developed approach to describe interatomic potentials in metals. The investigations show, for a realistic modeling of phase separation and coarsening processes in solder joints, such as for tin/lead alloys, the dependence of the stiffness matrix, the eigenstrains, and the surface tension on the concentration, play an essential role. This is due to the fact that both phases have different elastic properties as well as different expansion coefficients. For this reason, we focus on free energies with *concentration-dependent surface tension* and *elastic contributions*. The treatment of these additional dependencies is from a mathematical point of view, of course, more involved.

We consider a phase field energy functional of the following normalized structure:

$$E_\varepsilon(c,u) = \int_\Omega \Big(\varepsilon\sigma^2(c,\nabla c) + \frac{1}{\varepsilon}\psi(c) + W\big(c,\mathcal{E}(u)\big)\Big)dx, \qquad \varepsilon > 0, \tag{1}$$

where $\Omega \subset \mathbb{R}^n$ is the corresponding domain of the sample. The first summand in (1) represents *surface tension*, which penalizes rapid spatial variations in the concentration. Furthermore, this term is capable to model anisotropic effects depending on the concentration. The second term in the energy functional E_ε is the *chemical free energy density*. In the context of phase transitions, this energy density has usually the form of a double-well potential; see Figure 5. The function W is the elastic free energy density, where $\mathcal{E}$ is the strain tensor, and u denotes the displacement field.

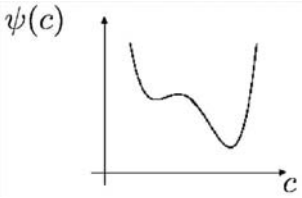


Fig. 5: *Chemical free energy density*

Chemical potential. One naturally associated quantity to the phase field energy is the chemical potential. It is defined as the functional derivative with respect to the concentration c:

$$w_\varepsilon = \frac{\delta E_\varepsilon}{\delta c} = 2\varepsilon\sigma(c, \nabla c)\,\nabla\cdot\sigma_{,p}(c, \nabla c) + 2\varepsilon\sigma(c, \nabla c)\,\sigma_{,c}(c, \nabla c) + \frac{1}{\varepsilon}\psi_{,c}(c) + W_{,c}(c, \mathcal{E}(u)).$$

Here, the indices c and p stand for partial derivatives with respect to the second variable c and the variable corresponding to ∇c.

The corresponding sharp interface model

We are now going to establish the sharp interface model that results from the phase field model if the transition layer becomes sharp. For the scaled phase field energy functional in (1), it can be shown that the width of the transition layer scales with order ε, and hence we obtain a sharp interface as $\varepsilon \to 0$.

Energy functional. In the asymptotic limit, the first two volume integrals of the phase field energy E_ε reduce to an area integral. The corresponding *sharp energy functional* is given by

$$E_0(c, u) = \int_I \sigma_0(\nu) d\mathcal{H}^{n-1} + \int_\Omega W\big(c, \mathcal{E}(u)\big)\, dx, \tag{2}$$

where the interface I is mathematically described by the reduced boundary of $\Omega_- := \{x \in \Omega : c(x) = c_-\}$, i.e., $I = \partial^*\Omega_-$, and ν denotes the outer unit normal of Ω_-. The anisotropy function $\sigma_0 : \mathbb{R}^n \to \mathbb{R}$ has the form

$$\sigma_0(p) = 2\int_{c_-}^{c_+} \sqrt{\psi(s)}\,\sigma(s, p) ds\,, \tag{3}$$

which models directionally-dependent surface tension effects.

Gibbs–Thomson law. The main reason for considering sharp interface limits is to deduce, from the phase field approach, jump conditions for local quantities like the chemical potential at the phase boundary in the sharp limit. This information enables us to switch from the phase field model to the sharp interface model and vice versa, depending on the aspects one wants to look at.

A weak formulation of a Gibbs–Thomson law with directionally dependent surface tension and elasticity has been rigorously established from the phase field approach in the sharp limit; see [3].

The Gibbs–Thomson law is derived by means of the first variation of the sharp energy functional. It states

$$w = \left(\nabla_I \cdot \sigma_{0,p} + \nu[W Id - (\nabla u)^T W_{,\mathcal{E}}]^+_- \nu\right)/(c_+ - c_-) \qquad \text{on} \quad I, \tag{4}$$

where w is the chemical potential, ∇_I denotes the tangential derivative, $W_{,\mathcal{E}}$ is the partial derivative with respect to $\mathcal{E}$, and $[\cdot]^+_-$ stands for the jump of the quantity in brackets at the interface. The second summand in (4) is the Eshelby traction.

Equation (4) is an extension of the classical Gibbs–Thomson law, which considers only the isotropic surface tension σ and no elastic effects. It relates the geometry of the phase boundary to the chemical potential w, i.e.,

$$w = \sigma\kappa \qquad \text{on} \quad I,$$

where σ is the constant surface tension; cf. [6].

Finally, we like to emphasize that we give in [3] a weak formulation of (4) in the sharp limit, involving only bulk contributions of the elastic terms, since in general not enough regularity is known for the deformation field. Our results are based on a generalized total variation of functions of bounded variation, on weak convergence theorems for homogenous functions of measures, and the construction of suitable approximants for phase field quantities and sharp interface quantities at the same time.

References

[1] T. Böhme, W. Dreyer, W. Müller, *Determination of stiffness and higher gradient coefficients by means of the embedded atom method: An approach for binary alloys*, Contin. Mech. Thermodyn., **18** (2007), pp. 411–441.

[2] C.M. Filho, M. Brizoux, H. Frémont, Y. Danto, *Improved physical understanding of intermittent failure in continuous monitoring method*, Microelectronics Reliability, **46** (2006), pp. 1886–1891.

[3] H. Garcke, C. Kraus, *An extended Gibbs–Thomson law arising from variational problems with general singular perturbations and elasticity*, to appear as WIAS Preprint.

[4] P.G. Harris, K.S. Chaggar, M.A. Whitmore, *The effect of ageing on the microstructure of 60:40 tin-lead solders*, Soldering & Surface Mount Technology, **3** (1991), pp. 20–33.

[5] D.J.C.K. Kwak, *The sharp-interface limit of the Cahn–Hilliard system with elasticity*, Ph.D. Thesis, Universität Regensburg, 2007.

[6] L. Luckhaus, L. Modica, *The Gibbs–Thompson relation within the gradient theory of phase transitions*, Arch. Rat. Mech. Anal., **107** (1989), pp. 71–83.

2.3 Optimal Control of Partial Differential Equations with Pointwise State Constraints

Christian Meyer

Numerous technical processes can be described by partial differential equations (PDEs). Prominent examples are the Navier–Stokes equations and Maxwell's equations that model fluid flows and electromagnetic processes, respectively. In the majority of cases, these equations cannot be solved analytically, but call for a *numerical simulation*. The solution of such processes by simulation is meanwhile well established in practice based on sophisticated discretization techniques for the underlying PDEs. In the recent past, the simulation-based *optimization* of technical systems governed by PDEs has therefore become a field of growing interest. Although significant progress has been achieved in this field concerning theoretical as well as algorithmic and numerical aspects, there are still a number of open questions, in particular for problems with so-called *pointwise state constraints*. Problems of this type are of major importance in various applications. We mention, for instance, the hardening of steel workpieces by heat treatment, where melting of the material has to be prevented, which mathematically corresponds to a pointwise state constraint. The goal of this article is to review the research at WIAS in the field of state-constrained optimal control of PDEs in the last years.

A stated-constrained model problem

For a brief introduction to the subject, let us consider a model problem that exhibits pointwise state constraints. The optimization is subject to *Poisson's equation*, which is a *linear elliptic* PDE of second order given by

$$-\Delta y := -\frac{\partial^2 y}{\partial x_1^2} - \frac{\partial^2 y}{\partial x_2^2} - \frac{\partial^2 y}{\partial x_3^2} = u \quad \text{in } \Omega, \tag{1}$$

where Ω denotes a given domain. On the boundary of Ω, denoted by Γ, *homogenous Dirichlet boundary conditions*, i.e., $y = 0$ on Γ, are imposed. A possible physical background for this PDE is the stationary heat equation in a solid body occupying the domain Ω. In this case, the solution of (1) represents the temperature distribution y induced by a distributed heat source u. In our context, the right-hand side u represents the *control*, which can be directly influenced. The solution y of (1) for given u is called the *state*. The aim of the optimization is to adjust the control u such that the difference between the actual and a desired state is as small as possible. This difference is measured by the *objective functional* J, which is to be minimized and possesses a quadratic structure in our case. In this way, one arrives at a so-called *linear-quadratic elliptic*

optimal control problem with pointwise state and control constraints, which reads as follows:

$$\left.\begin{aligned} \text{minimize} \quad & J(y,u) := \frac{1}{2}\int_\Omega |y-y_d|^2\,dx + \frac{\alpha}{2}\int_\Omega u^2\,dx\,, \\ \text{subject to} \quad & -\Delta y = u \quad \text{in } \Omega\,, \\ & y = 0 \quad \text{on } \Gamma\,, \\ \text{and} \quad & y_a(x) \le y(x) \le y_b(x) \quad \text{a.e. in } \Omega\,, \\ & u_a(x) \le u(x) \le u_b(x) \quad \text{a.e. in } \Omega\,. \end{aligned}\right\} \tag{P}$$

Here, y_d is a desired state, in our example a desired temperature that covers advantageous features for the respective application. Besides the difference between actual and desired state, the objective functional also contains the L^2 norm of the control u. This term reflects the wish to reach the desired state with minimum effort and is balanced by the positive parameter α. In addition, inequality constraints are imposed on control and state by given bounds u_a, u_b, and y_a, y_b. The first are referred to as *(pointwise) state constraints*, while the latter are called *(pointwise) control constraints*. In the case of the heat equation, the additional state constraints, i.e., $y_a(x) \le y(x) \le y_b(x)$ a.e. in Ω, may reflect the need to prevent melting or freezing. Moreover, the control constraints allow to incorporate threshold values for the heating power into the model. Due to the simple structure of the PDE, problem (P) is not sufficient for many applications, and physically reasonable problems exhibit more involved PDEs, as we will see below. Nevertheless, owing to the presence of pointwise state constraints, (P) already contains one of the main challenges of real-world optimal control problems.

Besides the questions of existence and uniqueness of an optimal solution for (P), one of the main tasks in the discussion of (P) is to find a suitable characterization of the optimal solution by means of *optimality conditions*. A crucial question in this context is to show the existence of so-called *Lagrange multipliers* associated with the inequality constraints in (P). These Lagrange multipliers allow for the formulation of optimality conditions, which can be used to numerically solve the optimization problem.

The theory of optimality conditions for problems of type (P) is meanwhile well established; see for instance [1] and also the recent monograph [6]. The underlying analysis is based on classical results for abstract optimization problems in Banach spaces. However, the application of these results requires to consider the state constraints in the space of continuous functions, denoted by $C(\bar\Omega)$. This fact leads to far-reaching consequences, since the associated Lagrange multiplier is then an element of the dual space $C(\bar\Omega)^*$, which is isomorphic and isometric to the space of *regular Borel measures*. Thus, the Lagrange multipliers associated with pointwise state constraints are in general *no proper functions, but only measures*.

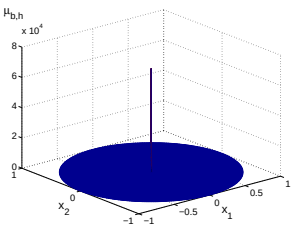


Fig. 1: *Example for a measure-valued Lagrange multiplier*

This lack of regularity of the Lagrange multipliers is also observed in numerical computations. Figure 1 shows the numerical approximation of a Lagrange multiplier for a state-constrained problem of the form (P). The picture is taken from [4]. The particular example is constructed in such a way that the exact Lagrange multiplier is given by a point measure in the origin. We observe that the discrete multiplier approximates this measure.

The low regularity of the multiplier impairs the regularity of the optimal control and the optimal state. We are thus faced with substantially more irregular solutions in the presence of state constraints compared to the purely control-constrained case or the case without any additional inequality constraints, respectively. This fact clearly complicates the numerical analysis and development of optimization algorithms for state-constrained problems. Nevertheless, it is possible to solve these problems numerically and to derive error estimates for their discretization, as demonstrated in the following.

Numerical approximation of elliptic problems with state constraints

For a numerical approximation of (P), one needs to discretize the optimal control problem on a given computational grid of mesh size $h > 0$. This can, for instance, be done by applying a standard *finite element* discretization to the elliptic PDE in (P), and by discretizing the control by means of *piecewise constant or piecewise linear ansatz functions*. The resulting discrete counterpart to (P) is a *finite-dimensional optimization problem*. Provided that the mesh size, and thus the number of unknowns, is not too large, the discrete problem can be solved by standard optimization methods, which are available in various common mathematical software packages. For the reliability of this standard approach, *a priori error estimates* for the approximation error for optimal control and state are indispensable.

Such error estimates were derived in [3] for a general class of linear-quadratic elliptic problems with state constraints. In the case of (P), the final estimate reads

$$\|\bar{u} - \bar{u}_h\|_{L^2(\Omega)} + \|\bar{y} - \bar{y}_h\|_{H^1(\Omega)} \le c\, h^{2-d/2-\varepsilon} \quad \text{with} \quad \varepsilon > 0, \tag{2}$$

where $(\bar{u}, \bar{y})$ denotes the optimal solution of the infinite-dimensional problem, while $(\bar{u}_h, \bar{y}_h)$ is the discrete optimal solution associated with the mesh size h. Moreover, d denotes the spatial dimension of the domain Ω, so that one obtains almost linear convergence in the two-dimensional case. It should be noted that the derived order of convergence is *optimal*. Better results cannot be expected due to the low regularity of the solution.

Remarkably, the predicted order of convergence is also observed in several numerical tests. Here, we refer to an example given in [3]. In this test case, the desired state is equal to one, and the lower bound y_a in the state constraints is constructed in such a way that it exceeds the desired state in some part of the computational domain; cf. Figure 2. The finite-dimensional optimization problem arising after the discretization is solved by using a *primal-dual path-following interior point method*, and we refer to [3] for a detailed description of this algorithm.

The computed optimal state for a mesh size of $h/\sqrt{2} = 0.02$ is shown in Figure 3. Observe that the optimal state tends to the desired state and obeys the lower bound at the same time.

The orders of convergence found experimentally in this example are depicted in Table 1. They were computed by a comparison of the numerical solution on a fine mesh with approximately two million nodes with solutions on coarser meshes; see [3] for details.

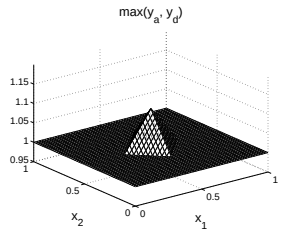


Fig. 2: *Lower bound and desired state*

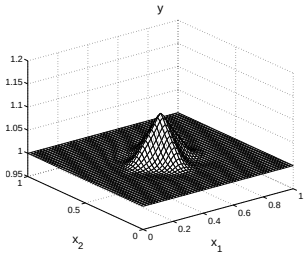


Fig. 3: *Optimal state*

Table 1: *Experimental order of convergence for a state-constrained optimal control problem*

h	1/80	1/100	1/120	1/140	1/160	1/180
$EOC_2(u)$	0.9324	1.0383	1.0886	1.1196	1.0838	1.0692
$EOC_{1,2}(y)$	1.0107	0.8674	1.3447	0.6220	1.6797	1.1445

Here, $EOC_2(u)$ refers to the experimental order of convergence for the L^2 error of the control, whereas $EOC_{1,2}(y)$ denotes the experimental order of convergence for the H^1 error of the state. We observe that both quantities average approximately one, and thus the numerical findings agree with the theoretical predictions in (2).

Two applications with state constraints

The model problem (P) is clearly artificial due to the simple structure of the associated PDE. However, it already provides the essential difficulty of state-constrained problems, since the Lagrange multipliers turn out to be measures in general, as seen above. This is also one of the most challenging issues in the investigation of application-driven optimal control problems containing more involved PDEs. In the following, we will illustrate this effect by two examples.

Optimal control of the thermistor problem. The first application covers the heat treatment of steel workpieces by direct current. This procedure is applied in automotive industry for the hardening of gear racks as part of the widely-used rack and pinion steering. The principal setup of this type of steering is shown in Figure 4.

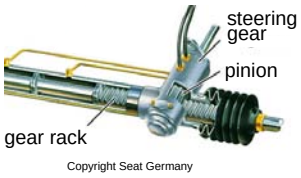


Fig. 4: *A rack and pinion steering*

During the hardening procedure, the workpiece is heated up by a direct current and then rapidly cooled down by means of water nozzles. In this way, a hard outer layer is produced that consists of a particular microstructure of steel called *martensite*. The aim of the optimization is a uniform heating of the teeth of the gear rack, which is essential for the hardening process in order to avoid thermal stress and to guarantee a uniform hardening of the tooth system.

The mathematical model for the heating of a conducting material by a direct current is given by the so-called *thermistor problem*. It consists of the *instationary heat equation* for the temperature θ and the *quasi-static potential equation* for the electric potential φ. To be more precise, the PDE for θ is given by the following *parabolic* equation, which describes the evolution of the temperature field in time and space.

$$\partial_t\theta - \operatorname{div}(\kappa\nabla\theta) = \sigma(\theta)(\nabla\varphi)^2 \qquad \text{in } Q := \Omega\times]0,T[, \tag{3a}$$

$$\nu\cdot\kappa\nabla\theta + \alpha\theta = \alpha\theta_e \qquad \text{on } \Sigma := \partial\Omega\times]0,T[, \tag{3b}$$

$$\theta(0) = \theta_0 \qquad \text{in } \Omega. \tag{3c}$$

Here, Ω is the domain covered by the conductor, and $\partial\Omega$ is its boundary with outward normal vector ν. Moreover, T is a given end time. In addition, κ, σ, α are material parameters, and θ_0 and θ_e denote initial and external temperature, respectively. In contrast to (1), the inhomogeneity in (3a) does not represent the control, but is given by the so-called *Joule heat sources* involving the electric potential φ. This quantity arises as solution of a further equation, which is an *elliptic* PDE

and reads as follows:

$$-\operatorname{div}(\sigma(\theta)\nabla\varphi) = 0 \qquad \text{in } Q, \tag{4a}$$

$$\nu \cdot \sigma(\theta)\nabla\varphi = u \qquad \text{on } \Sigma_N := \Gamma_N \times]0, T[, \tag{4b}$$

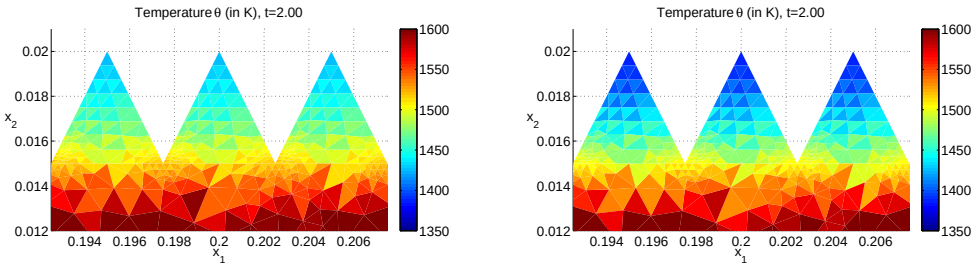
$$\varphi = 0 \qquad \text{on } \Sigma_D := \Gamma_D \times]0, T[, \tag{4c}$$

$$\nu \cdot \sigma(\theta)\nabla\varphi = 0 \qquad \text{on } (\partial\Omega \setminus \overline{\Gamma}_N \cup \Gamma_D) \times]0, T[. \tag{4d}$$

This equation models the electromagnetic features of the problem. The control is given by the *electric current* u induced at the cathode, i.e., the part Γ_N of the boundary $\partial\Omega$; see (4b). In contrast to this, one has homogeneous Dirichlet boundary conditions at the anode Γ_D and insulation on $\partial\Omega \setminus \overline{\Gamma}_N \cup \Gamma_D$.

As indicated above, the objective is to adjust the induced current u in order to achieve a temperature distribution that is as uniform as possible in the tooth system at end time T. At the same time, one has to obey pointwise state constraints, because the temperature must not exceed the melting temperature at any point and time, since it is essential to prevent melting during the hardening process. Together with the nonlinear coupling of (3a) and (4a), and the mixed boundary conditions in (4b)–(4d), these pointwise state constraints represent the most challenging feature of this particular optimal control problem.

As mentioned above, pointwise state constraints require the continuity of the state, which is the case for the temperature in the thermistor problem. The continuity of θ with respect to space and time was shown in [2]. Similarly to (P), the continuity of θ allows to prove the existence of Lagrange multipliers and to derive optimality conditions suitable for optimization algorithms.



(a) Optimization *without* state constraints

(b) Optimization *with* state constraints

Fig. 5: *Temperature distribution at end time*

In [2], such an algorithm was tested for the application-driven example of hardening a gear rack. The state-constrained optimization of an artificial two-dimensional gear rack was compared to the solution of a corresponding optimal control problem without state constraints. The results are depicted in Figure 5. The aim of the optimization was a uniform temperature of 1500 K in the teeth at $T = 2.0$ s. To prevent melting, the state constraints were given by $\theta(t, x) \leq 1800$ K for all $(t, x) \in Q$. Figure 5 shows the optimized temperature distribution at end time when the state constraints are neglected (a) and imposed (b), respectively. We observe that the result in the case without additional state constraints is closer to the desired state.

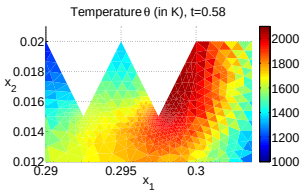


Fig. 6: *Temperature at $t = 0.58$ s in the case without state constraints*

However, in this case the material will melt, since the temperature exceeds the melting temperature of 1800 K; cf. Figure 6. In contrast to this, the algorithm yields a maximum temperature of 1805.1 K in the case of the state-constrained optimization, so that melting is indeed prevented.

Optimal control of sublimation growth of semiconductor single crystals. Another optimal control problem, where state constraints play an important role, is the optimization of sublimation crystal growth. This application was studied in close cooperation within the MATHEON project C9 "Numerical simulation and control of sublimation growth of semiconductor bulk single crystals" (see also page 96). It deals with the sublimation growth of semiconductor single crystals. The principle setup of a corresponding growth device consists of a growth crucible with a cavity inside. At the bottom of the cavity, polycrystalline powder is heated up until it sublimates and recrystallizes at the cooled top of the cavity. In this way, the desired single crystal grows into the reaction chamber.

In addition to more sophisticated models of sublimation growth studied in WIAS's Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*, we focused on a substantially simplified model. It only accounts for the stationary temperature distribution in the growth crucible and assumes that one can directly control the induced heat sources. The overall system is given by the *elliptic* PDE

$$-\mathrm{div}(\kappa_s \nabla\theta) = u \qquad \text{in } \Omega_s\,, \tag{5a}$$

$$-\mathrm{div}(\kappa_g \nabla\theta) = 0 \qquad \text{in } \Omega_g\,, \tag{5b}$$

$$\kappa_g \left(\frac{\partial\theta}{\partial n_r}\right)_g - \kappa_s \left(\frac{\partial\theta}{\partial n_r}\right)_s = G(\theta) \qquad \text{on } \Gamma_r\,, \tag{5c}$$

$$\kappa_s \frac{\partial\theta}{\partial n} + \varepsilon\sigma\,|\theta|^3\theta = \varepsilon\sigma\,\theta_e^4 \qquad \text{on } \partial\Omega_s, \tag{5d}$$

where Ω_s is the domain of the growth crucible with the cavity Ω_g inside. The interface between Ω_s and Ω_g is denoted by Γ_r. While θ is again the temperature distribution, the control u is in this case given by the heat sources in Ω_s. Furthermore, θ_e is a given external temperature, and κ_s, κ_g, ε, and σ are fixed material parameters. Due to the extremely high temperatures in this application, it is essential to account for *radiation* effects in this model. On the outer boundary $\partial\Omega_s$, this leads to so-called *Boltzmann radiation boundary conditions*. On the interface Γ_r, the radiation is *nonlocal*, since the incoming radiation at each point on Γ_r consists of the emission of every other point on Γ_r. Mathematically, this is modeled by the nonlinear integral operator G, which represents one of the challenges of the problem.

When optimizing this process, one aims at flat temperature gradients inside the reaction chamber Ω_g to improve the quality of the grown crystals. In addition, pointwise state constraints on the temperature are essential to ensure sublimation of the material and crystallization of the desired semiconductor single crystal.

In [5], we established continuity of the temperature field and, based on this, existence of Lagrange multipliers and optimality conditions for the associated state-constrained optimal control problem. Again, the Lagrange multipliers associated with the state constraints are in general measures, which is also confirmed by numerical computations. Figure 7 shows the Lagrange multiplier asso-

ciated with one of the different state constraints on the temperature. As in the other examples, we observe that the multiplier exhibits a significantly irregular structure.

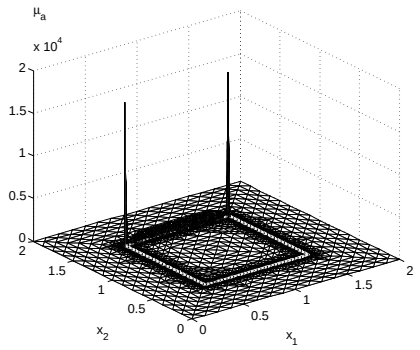


Fig. 7: *Lagrange multiplier associated with a state constraint within optimization of sublimation crystal growth*

Conclusion and outlook

State-constrained optimal control problems exhibit particular difficulties due to the low regularity of the associated Lagrange multipliers. Our examples show, in addition, that irregular multipliers do not only occur in pathological cases, but also in generic, application-driven optimal control problems. Nevertheless, it is possible to solve these problems by means of specialized optimization algorithms. Furthermore, it is in the case of linear-quadratic problems even possible to analyze the convergence of these algorithms and to prove a priori error estimates for the discretization of the infinite-dimensional optimization problems. One of the most challenging tasks in the near future is to transfer these results to nonlinear problems such as the optimal control of the thermistor problem and of sublimation crystal growth, respectively.

References

[1] E. Casas, *Boundary control of semilinear elliptic equations with pointwise state constraints*, SIAM J. Control Optim., **31** (1993), pp. 993–1006.

[2] D. Hömberg, C. Meyer, J. Rehberg, W. Ring, *Optimal control of the thermistor problem*, WIAS Preprint no. 1363, 2008.

[3] C. Meyer, *Error estimates for the finite-element approximation of an elliptic control problem with pointwise state and control constraints*, Control Cybernet., **37** (2008), pp. 51–85.

[4] C. Meyer, U. Prüfert, F. Tröltzsch, *On two numerical methods for state-constrained elliptic control problems*, Optim. Methods Softw., **22** (2007), pp. 871–899.

[5] C. Meyer, I. Yousept, *State-constrained optimal control of semilinear elliptic equations with nonlocal radiation interface conditions*, to appear in: SIAM J. Control Optim.

[6] P. Neittaanmäki, J. Sprekels, D. Tiba, *Optimization of Elliptic Systems: Theory and Applications*, Springer, New York, 2006.

2.4 Multiple Merger Coalescents in Population Genetics

Matthias Birkner

Populations, genetic variation, and genealogies

Fig. 1: *Sewall Wright (1889–1988), top image, and Sir Ronald Aylmer Fisher (1890–1962), bottom image, differed by approximately* 3×10^6 *mutations*

On the genetic level, there is considerable variation within most biological populations. For example, two "randomly picked" humans will typically differ at approximately three million positions of their genome. This may sound tremendous, but recall that the human genome consists of very long pieces of DNA sequence, altogether approximately 3×10^9 base pairs. Indeed, biologically, all humans are one population. Understanding the mechanisms leading to the genetic variability observed in living populations is sometimes quite rightly dubbed the "Great Obsession of population geneticists" (see [6], which also provides a very readable introduction to population genetics).

Beginning with the ground-breaking work of Charles Darwin, it has become understood that the genetic variability within populations drives and is being driven by *evolution*. The major evolutionary forces are mutation, selection, recombination, and genetic drift. *Mutation* refers to the fact that occasionally there are "copying errors" in the transmission of genetic information from parent to child. Broadly, *selection* denotes situations where a genetic type conveys (possibly quite indirectly) an advantage in reproductive success to its bearers, *recombination* is the mechanism of reassembly of maternal and paternal genetic material during the formation of gametes (egg and sperm cells) in sexual species. *Genetic drift* denotes the phenomenon that the genetic type composition in a finite population varies in time due to randomness in the reproduction, even in the absence of selective differences of the types.

Mathematical models are essential for the understanding of evolutionary processes and the interpretation of population genetic data. Since evolution acts so slowly that, in most cases, human observers cannot see it "in action", one usually has to take a retrospective viewpoint: Given observed genetic types in a (random) sample from the focal population today, one tries to infer parameters governing the evolution of this population, like the mutation rate at the observed genetic locus, historic population size, or parameters related to demographic variability (see below). As mutation, recombination, and genetic drift are intrinsically random processes, *stochastic* models are appropriate, and the retrospective viewpoint also poses a statistical problem.

In this article, we will focus on so-called *neutral* genetic variation, where the genetic type does not influence the individual's reproductive success. While selection is arguably the most interesting evolutionary force, neutral mutations are frequent: Synonymous mutations (due to redundancy in the genetic code) and mutations in noncoding regions are (at least to a good approximation) neutral. For example, the vast majority of *single nucleotide polymorphisms* in humans is believed to be neutral. Neutral genetic variation can thus form a useful marker to infer evolutionary parameters, but stochastic effects are much more pronounced than under selection. With neutral variation, genetic drift becomes the dominant effect. For simplicity, we will also only consider so-called *haploid* models, where the additional effects of sexual reproduction are ignored (nonetheless, such models can be used for sexual species with appropriate adjustments; see, e.g., [6]).

A conceptually very convenient property of neutral genetic types is the fact that it allows to disentangle (at least in a "gedankenexperiment") the usually unknown genealogy connecting the sampled individuals and their genetic types. In fact, one can start with a (stochastic) model for the reproduction of the individuals of the population; here, the paradigm model is the so-called *Wright–Fisher model* (see Figure 2), named for Sewall Wright and Sir Ronald A. Fisher, two of the "founding fathers" of mathematical population genetics. Then, in a second step, superimpose the genetic types of the individuals (and possibly mutations). For the distribution of the types observed in the sample, it will even suffice to superimpose types and mutations only along the genealogical tree connecting the sample (see Figure 6 for a schematic illustration).

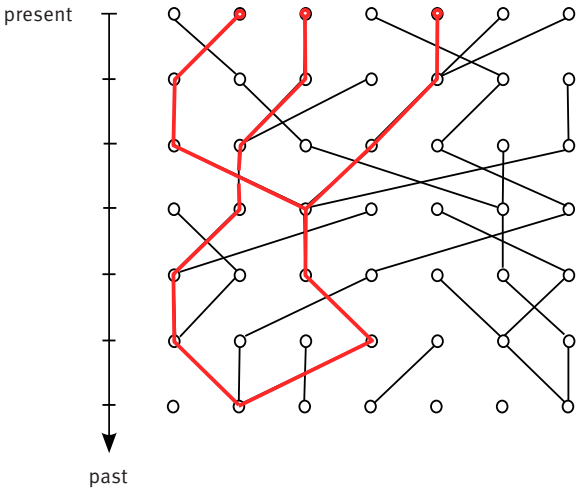


Fig. 2: *In the idealized dynamics of the Wright–Fisher model, each individual picks a "parent" randomly from the previous generation (depicted by a line in the image on the left). The genealogy of three individuals sampled from the present (topmost) generation is highlighted in red*

Note that Figure 2 also illustrates the effect of genetic drift: Only two of the seven individuals in the lowest generation have offspring in the topmost generation. Thus, at least in the absence of mutations, genetic types carried by the other individuals would be lost.

Kingman's coalescent. The standard, and very fruitful, approach in population genetic analyses is to take a backwards point of view and model the unknown genealogy connecting the sampled individuals as a random tree, whose distribution is determined by evolutionary parameters of interest. The "standard" model in this context is Kingman's coalescent (introduced by J.F.C. Kingman in 1982), which describes on appropriate time scales the random genealogies of a large class of population models (which generalize the Wright–Fisher model) in the limit of large population size. It is a "robust" model in the sense that only the asymptotic variance of the individual offspring number enters as a parameter in the limit, and has over the last 25 years been adapted to more general situations, involving, for example, (weak) selection, recombination, population expansion, or substructure. A key notion is the *effective population size* N_e, which replaces the census population size in coalescent-based calculations. Furthermore, based on Kingman's coalescent, efficient inference procedures for parameters of interest, such as (scaled) mutation rate, selection coefficients, or recombination rate have been investigated and implemented. A salient feature of models in the domain of attraction of Kingman's coalescent and its ramifications is that, at least in the limit of large population size, only *binary* mergers of ancestral lineages are visible (see Figure 3). This is

owed to the fact that the number of any individual's offspring must be negligible in comparison with the total population size.

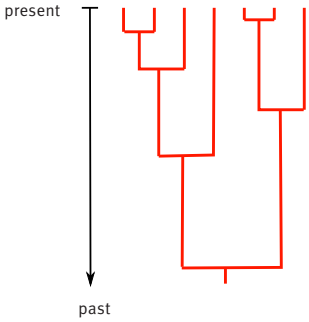


Fig. 3: *A realization of Kingman's coalescent. Each pair of lineages coalesces at rate* 1

Multiple merger coalescents. In 1999, more general coalescent processes have been "invented" (independently) by J. Pitman and by S. Sagitov. These coalescents allow multiple mergers of ancestral lineages. They can be biologically relevant in scenarios in which the variance of the number of offspring per individual is extremely large (recall that this variance enters as a parameter in the time scaling of Kingman's coalescent, which "breaks down" when the parameter becomes infinite): Occasionally, a single family forms a non-negligible fraction of the total population.

This may be expected, e.g., in species with a high individual reproductive potential in the face of high mortality early in life, like many marine species. Here, small variations in the local environment or simply temporal random fluctuations have the potential to drastically increase the variability of individual offspring numbers. In fact, it is known that the observed genetic variability in some marine organisms does not fit well to the predictions of Kingman's theory (see, e.g., [1], [5], and also the illustrations with a dataset from Atlantic cod below). Similar phenomena can be expected if the species under consideration experiences frequent local catastrophes followed by quick recolonization.

The dynamics of a Λ-coalescent is encoded by the eponymous Λ, which is a positive finite measure on the unit interval $[0, 1]$, as follows: While there are b lineages, any k-tuple merges into one at rate

$$\lambda_{b,k} = \int x^{k-2}(1-x)^{b-k}\,\Lambda(dx).$$

This form of the transition mechanism is dictated by the *consistency condition* $\lambda_{b,k} = \lambda_{b+1,k} + \lambda_{b+1,k+1}$ (think of a sample of size $b+1$, and ignore sample no. $b+1$, then the dynamics of the remaining samples must be that of a sample of size b).

While mathematically natural, the full class of all Λ-coalescents is "too large" from a practical point of view, as it corresponds to the infinite-dimensional space of all probability measures on the unit interval. In terms of data based on a finite sample, an analysis in the full class would be prone to over-fitting. Furthermore, the biological interpretation of a general measure Λ would be unclear.

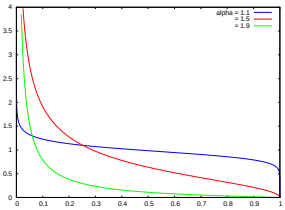


Fig. 4: *The* $Beta(2-\alpha,\alpha)$ *density for* $\alpha = 1.1$ *(blue),* $\alpha = 1.5$ *(red),* $\alpha = 1.9$ *(green curve)*

$Beta(2-\alpha,\alpha)$ coalescents. The family of $Beta(2-\alpha,\alpha)$ coalescents (a particular choice of the measure Λ, see Figure 4), where $\alpha \in (1, 2]$, constitutes particularly promising candidates: These coalescents arise as limits of genealogies of a class of neutral population models that generalize the Wright–Fisher model, where the probability that the individual litter size exceeds k decreases like $C \times k^{-\alpha}$ for some $C > 0$ (J. Schweinsberg, 2003). Thus, the family sizes have infinite (asymptotic) variance. The $Beta(2-\alpha,\alpha)$ class is also "mathematically" distinguished through a correspondence to branching processes via a suitable time change (Birkner et al., 2005), and it includes Kingman's coalescent as the boundary case $\alpha = 2$. Intuitively, the smaller α, the more skewed the offspring distribution, and the more frequent are extreme reproduction events.

The "forward" picture: Generalized Fleming–Viot processes. There is a more complete mathematical picture.

While the theory of Λ-coalescents takes a "retrospective" viewpoint, there is a corresponding *dual* stochastic process, the so-called Λ-*Fleming–Viot process*, which describes the evolution of the type composition in a population whose genealogies are given by a Λ-coalescent forward in time. This process is discontinuous: at rate $x^{-2}\Lambda(dx)$, a fraction x of the population dies and is replaced by the offspring of one individual. See, e.g., [3] for an overview.

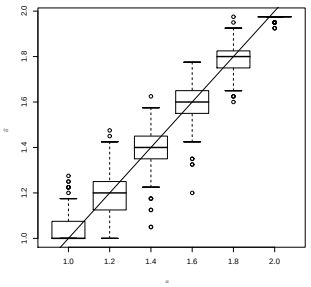


Fig. 5: *The offspring distribution tail parameter α can (in principle) be recovered from observations: Boxplots for the (empirical) distribution of the maximum likelihood estimator for α based on full genealogical information in a sample of size* 100

Likelihood computations

Mutations on a coalescent. Think of the observed genetic types as generated by superimposing mutation events at a certain *mutation rate* r on a Λ-coalescent (where the type of the root, the *most recent common ancestor* of the sample, is drawn from an equilibrium distribution), and then "read off" the types at the leaves (see Figure 6 for an example). From the point of view of inference of the parameters, e.g., the mutation rate r and the demographic parameter α, it is natural to compute the so-called *likelihood* (the probability of observing the data as a function of the parameters), and then maximize to find estimators.

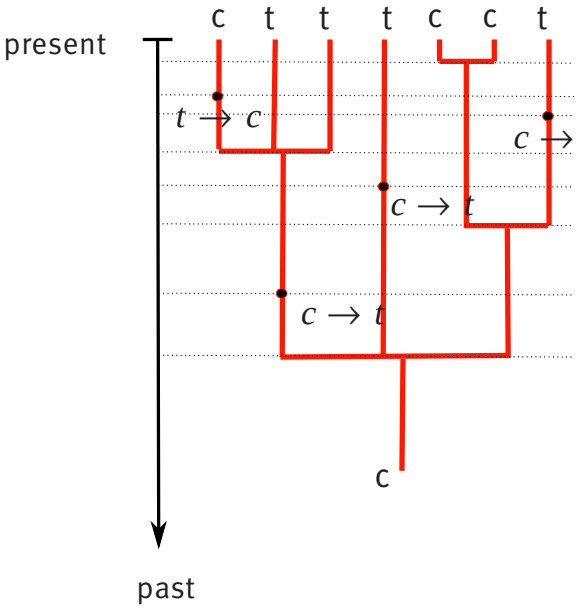


Fig. 6: *A multiple merger coalescent marked with mutations encodes the history of a sample: Letters at the leaves denote the genetic types of the samples, dotted lines correspond to time points of "events" in the history, black dots to mutations*

An urn scheme. The marked coalescent generates a *history* $\mathcal{H} = (H_{-\tau}, H_{-\tau+1}, \ldots, H_{-1}, H_0)$ of the sample (see Figure 6), where H_i records the ancestral state immediately after the i-th event and which lineage was split (and into how many) or which lineage mutated (and into which type), respectively, in the i-th event. For given n, Λ, and r, the sequence forms a Markov chain whose transition probabilities $\mathbb{P}^{(n)}_{\Lambda,r}(H_{i+1}|H_i)$ can be expressed explicitly in terms of r and the λ_{bk}; see

[2]. Thinking of lineages as "balls" and genetic types as "colors", this can be interpreted as a *random urn scheme*: in each step, one of the lineages is picked and either transformed (in a mutation event), or a random number of balls of the same color is added (a splitting event / coalescence event), where the respective probabilities can be computed as a function of n, Λ, r, and the current number of balls in the urn. Note that unlike the classical case corresponding to Kingman's coalescent, the transition probabilities *do* depend on the final sample size n.

In this formulation, the observation of certain types in a sample of size n corresponds to fixing a particular H_0.

Too big a sum. In principle, for given data D in a sample of size n, the desired likelihood $\mathbb{P}^{(n)}_{\Lambda,r}(D)$ can be computed by summing out all possible histories compatible with the observations

$$\mathbb{P}^{(n)}_{\Lambda,r}(D) = \sum_{\mathcal{H}:H_0=D} \mathbb{P}^{(n)}_{\Lambda,r}(\mathcal{H}) = \sum_{\mathcal{H}:H_0=D} \prod_{i=-\tau(\mathcal{H})}^{-1} \mathbb{P}^{(n)}_{\Lambda,r}(H_{i+1}|H_i). \tag{1}$$

However, direct summation is only feasible for very small sample sizes n, since the number of possible histories grows quickly with n.

A Monte Carlo method. One can try to approximate the sum in (1) by simulation: Draw R independent sample histories $\mathcal{H}^{(1)}, \ldots, \mathcal{H}^{(R)}$ according to the law $\mathbb{P}^{(n)}_{\Lambda,r}$ and record the empirical relative frequency of histories with $H_0 = D$. This naïve approach fails for moderate sample sizes, since typical likelihoods can be of the order 10^{-30}, so that too many replicates would be required.

Importance sampling provides a solution: We choose a law Q on histories which concentrates on histories that are compatible with data, simulate $\tilde{\mathcal{H}}^{(1)}, \ldots, \tilde{\mathcal{H}}^{(R)}$ according to Q and estimate

$$\mathbb{P}^{(n)}_{\Lambda,r}(D) = \mathbb{P}^{(n)}_{\Lambda,r}(\{\mathcal{H} : H_0 = D\}) \approx \frac{1}{R} \sum_{r=1}^{R} \frac{\mathbb{P}^{(n)}_{\Lambda,r}(\tilde{\mathcal{H}}^{(r)})}{Q(\tilde{\mathcal{H}}^{(r)})}.$$

Obviously, for the performance of this method, it is crucial to choose a "good" *proposal distribution* Q. The article [2], generalizing earlier work of R. Griffiths and S. Tavaré in the context of Kingman's coalescent, discusses a suitable Q and the ensuing Monte Carlo method for likelihood computations under Λ-coalescents. The program `beta genetree` implements the algorithm from [2]; it is freely available under the GNU General Public License from

`http://www.wias-berlin.de/~birkner/bgt/`

Illustration: Mitochondrial *cyt b* from the Atlantic cod

Fig. 7: *Atlantic cod (*gadus morhua*)*

We illustrate the use of `beta genetree` by estimating the (log-)likelihood surface in the α-r plane of a dataset consisting of genetic variation in the mitochondrial *cyt b* gene from 117 Atlantic cod (a subsample of the dataset described in [1]), analyzed under the *infinitely-many-sites model*, see Figure 8. The maximum likelihood estimator for α is $\widehat{\alpha} = 1.3$ and lies clearly away from the "Kingman axis" $\alpha = 2$, in keeping with the observations in [1].

	468	481	487	488	490	496	508	523	562	601	631	643	649	685	691
66	t	a	a	c	a	a	t	g	a	t	g	a	c	c	g
17	-	-	-	-	-	-	c	-	-	-	-	-	-	-	-
14	-	-	-	-	-	-	-	a	-	-	-	-	-	t	-
8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	t
1	-	-	-	-	-	-	-	-	-	-	-	-	-	t	-
2	-	-	-	t	-	-	-	-	-	-	-	-	-	-	-
1	-	-	-	-	-	-	-	a	-	-	-	g	-	t	-
1	-	-	-	-	-	-	-	-	-	-	-	-	t	-	-
1	-	-	-	-	g	-	c	-	-	-	-	-	-	-	-
1	-	-	-	-	-	g	-	-	-	-	-	-	-	-	-
1	-	-	g	-	-	-	-	-	-	-	a	-	-	-	t
1	-	-	-	-	-	-	c	-	g	-	-	-	-	-	-
1	g	-	-	-	-	-	-	-	-	-	-	-	-	-	-
1	-	-	-	-	-	-	-	-	-	c	-	-	-	-	-
1	-	c	-	-	-	-	c	-	-	-	-	-	-	-	-

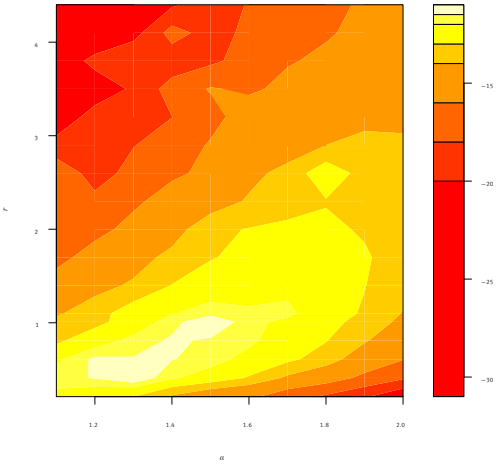


Fig. 8: *Left: Genetic variation at the mitochondrial* cyt b *locus in a sample of 117 Atlantic cod. Right: Estimated log-likelihood surface for this dataset*

References

[1] E. Árnason, *Mitochondrial cytochrome b DNA variation in the high-fecundity Atlantic cod: Trans-Atlantic clines and shallow gene genealogy*, Genetics, **166** (2004), pp. 1871–1885.

[2] M. Birkner, J. Blath, *Computing likelihoods for coalescents with multiple collisions in the infinitely-many-sites model*, J. Math. Biol., **57(3)** (2008), pp. 435–465.

[3] ———, *Measure-valued diffusions, general coalescents and population genetic inference*, to appear in: Trends in Stochastic Analysis, J. Blath, P. Mörters, M. Scheutzow, eds., Cambridge University Press.

[4] M. Birkner, J. Blath, M. Möhle, M. Steinrücken, J. Tams, *A modified lookdown construction for the Xi–Fleming–Viot process with mutation and populations with recurrent bottlenecks*, to appear in: ALEA Lat. Am. J. Probab. Math. Stat.

[5] B. Eldon, J. Wakeley, *Coalescent processes when the distribution of offspring number among individuals is highly skewed*, Genetics, **172** (2006), pp. 2621–2633.

[6] J. Gillespie, *Population Genetics: A Concise Guide*, Johns Hopkins Univ. Press, Baltimore, MD, 1998.

2.5 Leonid Shilnikov and the Unveiling of Deterministic Chaos

Matthias Wolfrum

Fig. 1: *Leonid P. Shilnikov, 2008*

The Alexander von Humboldt Foundation is nominating internationally outstanding foreign scientists whose fundamental discoveries have had a significant impact on their discipline for a Humboldt Research Award in order to promote the cooperation between excellent scientists from abroad and from Germany. The award winners are invited to spend a period of up to one year at a research institution of their choice in Germany. It has been a particular honor for the Weierstrass Institute to be among the hosting institutions for Leonid P. Shilnikov, laureate of the Humboldt Research Award, during his stay in Germany in 2008.

In fact, the beginning of the cooperation with L.P. Shilnikov and his group at the Institute for Applied Mathematics and Cybernetics in Nizhni Novgorod, Russia, dates back already more than ten years, when one of his former collaborators, D. Turaev, now full professor at the Imperial College in London, was a collaborator of WIAS for several years, and others of his collaborators were guests at WIAS.

L.P. Shilnikov's contributions indeed have had a significant impact on the development of applied mathematics in the second half of the 20th century. The terms *Shilnikov chaos*, *Shilnikov bifurcation*, or *Shilnikov homoclinic* are today not only known to mathematicians, but play an important role in many fields, as, e.g, in engineering, chemistry, weather forecast, and climate modeling. And in particular, they are also important for the understanding of the complicated dynamics of optoelectronic devices and semiconductor lasers that are in the focus of interest of the Research Group *Laser Dynamics* at WIAS. But instead of a detailed discussion of some recent results related to L.P. Shilnikov's work, we want to give here an outline of the basic concepts and some historical context of the development of these ideas in the second half of the 20th century.

What does chaotic motion in a deterministic system mean?

A *dynamical system* is the mathematical form of the principle of causality: The state of the system is described by some variables from a state space, and the time variation of the state is described by a functional dependence of the state variables on a time variable. The variations of the state variables are given by some law of motion taking the form of a differential equation that establishes a relation between the actual state of the system and its velocity of change. Different solutions of the differential equation then correspond to the motions of the system with different initial conditions.

The most simple dynamical behavior is a stable stationary solution where the motion is at rest or comes to rest after a transient motion from some initial condition that is different from the stationary state. Stationary states can also be unstable as, e.g., the upright position of a pendulum.

A motion that corresponds to the typically observed behavior of a real system has to be not transient and in some sense stable. There are many examples of stable periodic motions, for instance,

a dripping water tap, the heartbeat, or the motion of a planet. There exists also the notion of a quasiperiodic motion, meaning that there are several degrees of freedom oscillating at different and incommensurable frequencies. In this way, very complicated motions are possible, and this scenario has been used, for example, to explain turbulence in fluid mechanics. Also stochastic external disturbances can lead to the observation of complicated motions. But it has been discovered only in recent decades that an irregular, seemingly chaotic behavior with several other surprising properties can already be present in relatively simple and small systems, and there is still considerable research ongoing to develop this mathematical theory and its applications to other fields of science.

A brief excursion into history

The first hints of chaotic motions were already found by the French mathematician Henri Poincaré in the last decade of the 19th century, when he failed to find a proof for the stability of the solar system. Like most of the pioneers of deterministic chaos, he was not a pure mathematician in the classical sense but, trained as a mining engineer, much more interested in applications and practical consequences of mathematical theory. But his pioneering ideas on irregular motions were not further developed at that time and, even more, the field of low-dimensional ordinary differential equations was considered as a more or less well-understood part of mathematics. And so, when in 1927 the Dutch radio engineers B. van der Pol and J. van der Mark observed chaotic behavior in a simple electric circuit, they had no theoretical framework to explain their observations [1].

Fig. 2: *Henri Poincaré (1854–1912)*

The breakthrough came only several decades later. Like the finding of penicillin by Alexander Fleming in 1928, it was to a certain extent an accidental discovery. In 1963, the American meteorologist Edward Norton Lorenz (1917–2008) was solving a simplified hydrodynamical model on a computer. Repeating the same calculation with the same initial data some days later, he surprisingly found that the trajectory rapidly diverged from the one calculated before. It turned out that this was only due to a slight change in the initial data caused by a rounding error of less than 0.1 %, a difference that, as it was considered at that time, should not have had any substantial influence on the final result. Lorenz immediately realized the consequences of this observation. For the long-term weather forecast that he was dealing with, it would be necessary not only to have a perfect model of all physical processes involved, but also an absolutely exact knowledge of the initial data. Otherwise, the observed effect could lead to a completely different result after a relatively short time span [2]. Later, he illustrated his ideas in a talk with the title “Predictability: Does the Flap of a Butterfly’s Wing in Brazil Set Off a Tornado in Texas?”.

Already a short time after these results were published, L.P. Shilnikov, who was at that time working on nonlocal bifurcations, started to investigate these phenomena from a mathematical point of view. It was known that periodic solutions can transform into a homoclinic loop to a saddle point. A homoclinic loop is a closed trajectory, starting and ending at the same point in phase space, and describes a motion that tends both for infinite positive and negative time to the same stationary solution. In the case of a two-dimensional system, the periodic solution disappears after this transition, and no new stable structure emerges. Studying the same scenario in three dimensions, Shilnikov realized that at a homoclinic loop to a saddle focus the situation changes drastically. At

a saddle focus (see Figure 3), the motion towards the equilibrium is governed by a pair of complex conjugate eigenvalues $\lambda_{1,2} = -\rho \pm i\omega$, while the divergence in the remaining direction is governed by a single real eigenvalue $\lambda_3 = \gamma > 0$. This leads to a spiraling motion of the incoming homoclinic loop. It turned out that under the condition $\gamma - \rho > 0$, complicated dynamics appear in the vicinity of the homoclinic loop [3]. To overcome the difficulties in the mathematical treatment of this problem, Shilnikov invented a powerful technique for the description of the behavior near the equilibrium, now known as *Shilnikov coordinates*. In this way, he could show, in particular, the existence of infinitely many unstable periodic orbits in the vicinity of the homoclinic loop. In fact, the cross sections (shown in green in the figure) are mapped back onto themselves in a way that can be described by the so-called *Smale horseshoe map*, an example of a chaotic mapping introduced by S. Smale.

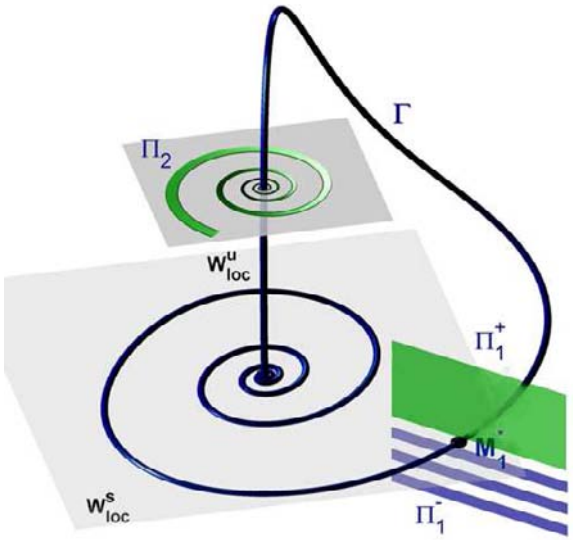


Fig. 3: *Shilnikov homoclinic orbit, inducing chaotic motion*

Today, deterministic chaos is usually characterized by three properties: Besides the sensitive dependence on initial data and an infinite set of dense periodic orbits, an abstract property, called *topological mixing*, is required. However, it took another decade until the term *chaos* was introduced into mathematics by the American mathematician J. Yorke in 1975, when he was dealing with iterated mappings of the unit interval. Later, computer-generated illustrations of chaotic attractors, impressing by their rich and fractal structure, became popular and contributed to the public awareness of chaos theory. However, concerning the relevance for real applications, Shilnikov's approach to chaos via homoclinic loops turned out to be the most successful. With modern methods of numerical path-follwing algorithms, the homoclinic loop and the related saddle quantities can be computed directly, and in this way, the emergence of chaos can be studied in many applied systems.

Transitions to chaos

Besides a detailed study of the chaotic dynamics themselves, for example, so-called *wild spiral attractors* [4], the formation of chaos during the transition from simple dynamics is a challenging mathematical problem. Dynamical systems with simple behavior are called *Morse–Smale systems* and form a subset in the space of all possible dynamical systems. Depending on the control parameters, a system may change its dynamical behavior. Such an event is called a *bifurcation*, since in simple cases, a new branch of solutions, e.g., a periodic solution, bifurcates from another solution. The boundary of Morse–Smale systems and the formation of chaos constitute a particularly complicated case of a bifurcation. After his first pioneering results, L.P. Shilnikov has been working on that question for many years. Major results in this direction were the transition to chaos through a non-transverse homoclinic to a periodic solution, and another case, where the chaotic dynamics arise after the disappearance of a periodic orbit of saddle-node type, the so-called *transition to chaos by intermittency*.

Jointly with D. Turaev, he has found more recently also a new type of bifurcation of a stable periodic solution [5], by a similar construction. After a list of four codimension-one bifurcations of stable periodic solutions has been known for a long time, it was an open question whether there is a bifurcation where the stable periodic solution disappears without interacting with a stationary state, i.e, into the “blue sky”. Figure 4 shows the scenario at the moment of disappearance of the stable periodic orbit. In addition to the primary periodic orbit, which is going to disappear, there is another periodic orbit of saddle-node type involved to which the primary periodic orbit becomes asymptotic for both positive and negative time. Performing in this way an increasing number of small oscillations in the vicinity of the saddle-node orbit, the period and the length of the primary periodic orbit tend to infinity at its disappearance.

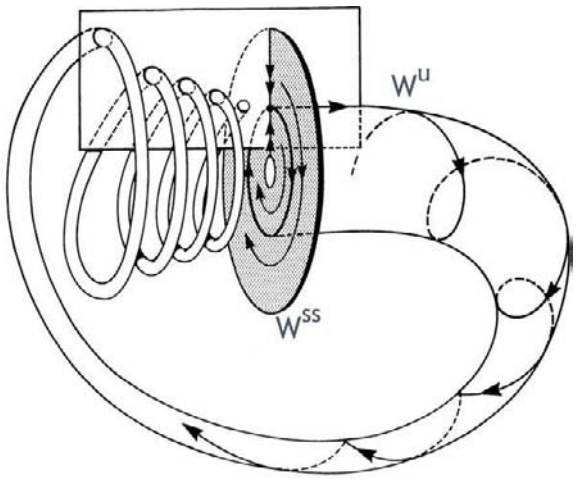


Fig. 4: *“Blue sky catastrophe”: A periodic orbit vanishes without interacting with a stationary state*

This bifurcation has turned out to play a central role in models from mathematical neuroscience, a field on which L.P. Shilnikov has been focusing his interest in recent years. During his visit to WIAS, L.P. Shilnikov shared his profound knowledge and experience in inspiring discussions with young scientists interested in this field of research. He gave several lectures and seminars also in the

framework of the DFG Collaborative Research Center "Complex Nonlinear Processes", where complicated dynamics in a variety of systems, ranging from cellular biology to semiconductor lasers, are investigated.

References

[1] B. van der Pol, J. van der Mark, *Frequency demultiplication*, Nature, **120** (1927), pp. 363–364.

[2] E.N. Lorenz, *Deterministic nonperiodic flow*, J. Atmospheric Sci., **20(2)** (1963), pp. 130–141.

[3] L.P. Shilnikov, *A case of the existence of a denumerable set of periodic motions*, Sov. Math. Dokl., **6** (1965), pp. 163–166.

[4] D.V. Turaev, L.P. Shilnikov, *An example of a wild strange attractor*, Sbornik Math., **189(2)** (1998), pp. 291–314.

[5] A. Shilnikov, L.P. Shilnikov, D. Turaev, *Shilnikov blue sky catastrophe in singularly perturbed systems*, Mosc. Math. J., **5(1)** (2005), pp. 205–218.

2.6 Numerical Simulations for Electrochemical Systems

Jürgen Fuhrmann

Electrochemical processes are ubiquitous in nature, science, and technology. We live due to ion channels in cell membranes. Ion transport causes corrosion and is the essential process in batteries and fuel cells. All these phenomena are rather complex. Adsorption/desorption reactions on catalyst surfaces, chemical reactions with electron transfer, and transport of molecules and ions compete in different ways in the above-mentioned examples.

The mathematical models describing these interactions are often formulated as partial differential equations. In particular, simple geometries permit the formulation of asymptotic models. These describe processes at high flow velocities. They are well suited to govern experimental designs to measure interesting quantities. On the other hand, these models are based on many simplifications with respect to geometry and the selection of the processes involved.

Computational methods permit a more general approach. These methods allow to approximate the continuum models by finite-dimensional models that can be solved by computers.

In the sequel, we describe two electrochemical applications that have been studied in the numerical analysis group of the Weierstrass Institute. The group uses the finite volume method based on Voronoi boxes. In the context of equations coupling convection, diffusion, and reactions, this method allows to connect geometric flexibility with a good representation of the underlying physics and chemistry [3].

Direct methanol fuel cells

Fuel cells are, like batteries and rechargeable batteries, electrochemical devices that convert chemically stored energy into electrical energy. An exothermal (combustion-like) chemical reaction is split into two spatially separated steps. At the anode of such a device, electrons are created in a catalytic reaction, flow through an outer circuit, and perform physical work. In the interior, an electrolyte allows for the exchange of ions between anode and cathode.

Batteries store the input substances in their volume and are “empty” if this reservoir is exhausted. Rechargeable batteries make it possible to reverse the reaction by applying an exterior voltage. Fuel cells are characterized by a continuous supply of the input substances and the removal of the reaction products. Hence, continuous operation and quick recharge are possible. Fuel cells mainly differ in the electrolyte used. Polymer electrolyte membrane fuel cells contain a proton-conducting polymer membrane (PEM), which typically consists of sulfonated polytetrafluorethylene (Nafion®). These membranes work at temperatures below 100°C and have to contain water to achieve a significant proton conductivity.

Mainly, hydrogen and methanol can be used as fuel. At room temperature, methanol is a liquid and has the advantage of easier storage, transport, and handling than gaseous H_2, while the latter exhibits more efficient reaction kinetics.

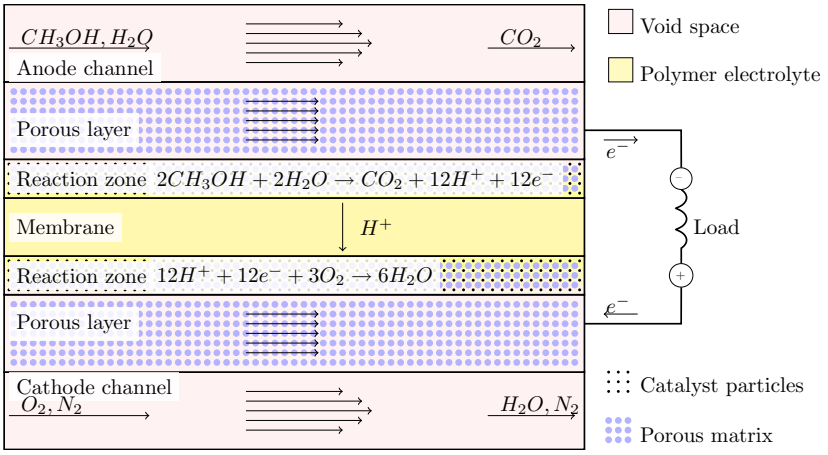


Fig. 1: *Schematic of a Direct Methanol Fuel Cell*

In a cooperation between WIAS and the Forschungszentrum (research center) Jülich, a 1D/2D/3D numerical model of a membrane electrode assembly has been developed that models the described physical processes by a system of coupled nonlinear partial differential and algebraic equations [2], [4]. Particular advantages of the model are the description of two-phase flow processes including a gas mixture and mixed wettability effects in the porous layers, and a detailed description of the electrocatalytic reactions. The choice of the finite volume method for space discretization allows geometric flexibility and ensures positive concentrations. Positivity of solutions is a special facet of the mathematical properties of the chosen discretization scheme.

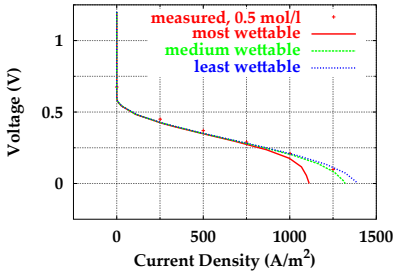


Fig. 2: *Dependence of the DMFC polarization curve on the wettability of the porous medium*

Using mainly data from literature, and fitting a few less well-known values, it was possible to adapt the model to measurements and to use it in order to interpret and predict a number of observations [2]. It is possible to describe the dependence of the cell performance on the porous media properties (see Figure 2), the efficiency losses due to the reaction kinetics, the transport phenomena, the poisoning of catalytic sites by CO, etc.

One problem intentionally left out in this model is the coupling of free flow and porous media flow at the interface between supply channel and porous transport layer. This problem is currently a topic of active research in several groups. At WIAS, the various options for a coupling of these processes are investigated with the aim to develop a finite volume approach to its solution that would supplement the methods developed so far.

Flow cells

Among other problems, the accuracy of this complex model is limited by the accuracy of available data. In order to gain deeper insight into particular electrochemical processes and to support the extraction of quantitative data, the group started cooperations with experimentalists working on flow cells.

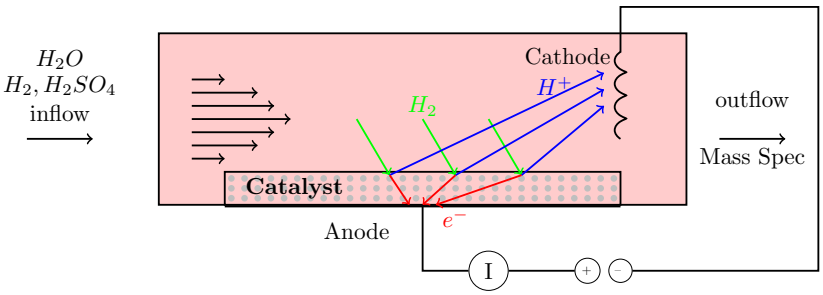


Fig. 3: *Schematic of a flow cell*

Thin-layer flow cells serve as experimental devices for the investigation of electrochemical processes. Being simpler than a fuel cell, they are easier to model and to understand. The final goal of this work is the quantitative understanding of all relevant steps in the electrochemical reaction chain.

In the easiest case of a flow cell, a solution containing sulphuric acid as an electrolyte and hydrogene as an electroneutral reactant is injected at a given rate at the inlet. At the anode, the H_2 molecules are catalytically oxidized, creating electrons and protons. The protons are transported to the cathode by the electrolyte, while the electrons reach the cathode in an outer circuit. The amount of hydrogen reacted is proportional to the electric current, which can be measured at the anode; for a schematic, see Figure 3. Instead of H_2, other substances may be fed at the inlet and their electrocatalytic reactions investigated. The reaction products can be analyzed by a mass spectrometer at the outlet.

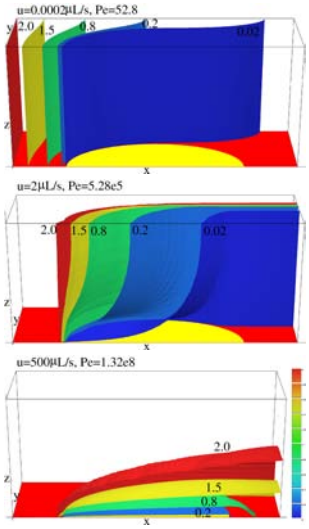


Fig. 4: *Isosurfaces of the concentration in a rectangular flow cell for different flow rates. The circular catalyst spot is shown in yellow at the bottom*

The simplest experiment that can be performed in a flow cell is the investigation of the limiting current, which flows if the anode reaction is fast in comparison to other processes. This is the case for hydrogen oxidation on platinum electrodes at appropriate voltage levels. The comparison between calculated and measured values of the limiting current therefore allows to benchmark the transport behavior of a flow cell. In order to model this behavior, two coupled physical processes are described by partial differential equations: the flow of electrolyte and the transport of a reactive species dissolved in it.

For channel-like structures, the fluid transport can be described by an analytical formula, while for more general geometries, the equations describing the fluid flow have to be solved numerically.

The transport problem is solved using the above-mentioned Voronoi box based finite volume method. Specific issues in solving the problem numerically are (a) mass conservation of the transported species; (b) an H_2 concentration greater than zero and not exceeding the inlet concentration; (c) a divergence-free velocity field.

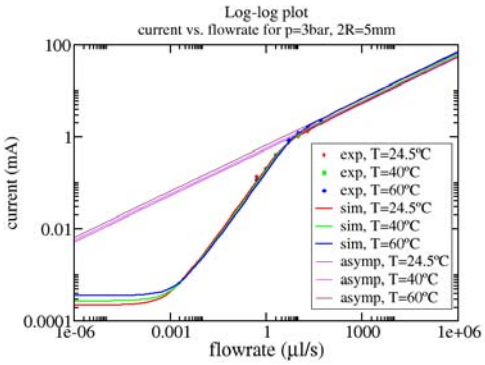


Fig. 5: *Comparison between fitted and measured values, and asymptotic approximations in a rectangular flow cell*

This approach has been applied to investigate the limiting current in a rectangular flow cell for different flow rates and temperatures. Using data from literature, a good qualitative agreement with measurements performed at the University of Ulm [6] was obtained. Diffusion coefficient and inlet concentration have been fitted to experimental data using our model, leading to a good agreement between simulation and measurement; see Figure 5.

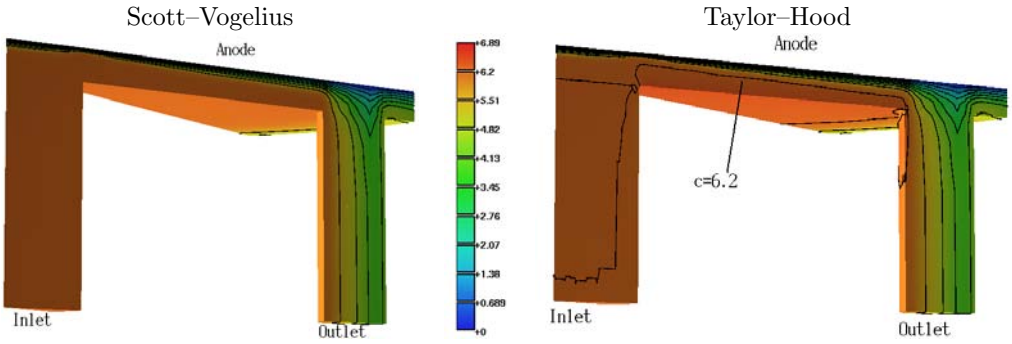


Fig. 6: *Left: The H_2 concentration in the cell is bounded by its value at the inlet when using the Scott–Vogelius element for the fluid flow. Right: The H_2 concentration in the cell exceeds its value at the inlet when using the Taylor–Hood element*

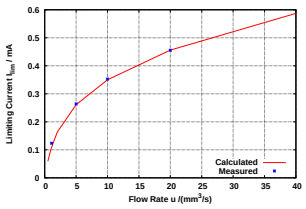


Fig. 7: *Measured and calculated values for the limiting current in a cylindrical flow cell*

According to the computations, the lower part of the measured flow rates is in a region where asymptotic models are not valid; see Figure 4. For these flow rates, the numerical model is the only possible way for a quantitative interpretation of the experimental results. For higher flow rates, we obtain a good coincidence with asymptotic expressions.

Often, one faces more general situations. Then, a numerical model is the only option to meet the practical requirements. In this case, condition (c) is guaranteed by the use of the Scott–Vogelius mixed finite element for the approximation of the fluid flow.

The convergence properties of this element have been investigated in [1]. Furthermore, a coupling scheme of the Voronoi box based finite volume method to this finite element scheme has been developed that solves problems (a) and (b). It has been applied to a cylindrical flow cell constructed at the University of Bonn [5]; see Figure 6.

Using the data obtained in [6], the measured limiting current data for the cylindrical flow cell have been successfully compared to calculated values, see Figure 7.

Outlook

Flow cells are used for qualitative and quantitative investigations of electrocatalytic multistep reactions. The undertaken modeling efforts allow to contribute to the understanding of such reaction processes by the help of numerical models. Such an understanding is essential for the improvement of the construction of a number of electrochemical applications, including fuel cells.

Acknowledgment

The project has been supported by the German Ministry of Education and Research within the framework "Netzwerke Grundlagenforschung für Erneuerbare Energien und Rationelle Energieanwendung" (Networks for basic research in renewable energies and efficient energy use) and by the DFG Research Center MATHEON "Mathematics for key technologies".

References

[1] E. BURMAN, A. LINKE, *Stabilized finite element schemes for incompressible flow using Scott–Vogelius elements*, Appl. Numer. Math., **58** (2008), pp. 1704–1719.

[2] J. DIVISEK, J. FUHRMANN, K. GÄRTNER, R. JUNG, *Performance modeling of a direct methanol fuel cell*, J. Electrochem. Soc., **150** (2003), pp. A811–A825.

[3] R. EYMARD, J. FUHRMANN, K. GÄRTNER, *A finite volume scheme for nonlinear parabolic equations derived from one-dimensional local Dirichlet problems*, Numer. Math., **102** (2006), pp. 463–495.

[4] J. FUHRMANN, K. GÄRTNER, *Modeling of two-phase flow and catalytic reaction kinetics for DMFCs*, in: Device and Materials Modeling in PEM Fuel Cells, S. Paddison, K. Promislow, eds., vol. 113 of Topics in Applied Physics, Springer, 2009, pp. 297–316.

[5] J. FUHRMANN, A. LINKE, H. LANGMACH, H. BALTRUSCHAT, *Numerical calculation of the limiting current for a cylindrical thin layer flow cell*, submitted.

[6] J. FUHRMANN, H. ZHAO, E. HOLZBECHER, H. LANGMACH, M. CHOJAK, R. HALSEID, Z. JUSYS, R. BEHM, *Experimental and numerical model study of the limiting current in a channel flow cell with a circular electrode*, Phys. Chem. Chem. Phys., **10** (2008), pp. 3784–3795.

2.7 Dewetting of Complex Liquids: Lubrication Models, their Analysis and Predictions

Georgy Kitavtsev (Institute of Mathematics, Humboldt University of Berlin) and Barbara Wagner

Dewetting thin films of complex liquids, such as liquid polymers, play an important role in numerous technological processes ranging from lithography to biological membranes. One major focus of interest is to understand the dynamics and morphology of polymer films dewetting from hydrophobic substrates, where the film thickness typically ranges on a scale of tens to a few hundred nanometers. The dewetting process starts by the formation of holes due to so-called *spinodal decomposition*, i.e., the breakup of the thin film due to tiny perturbations of the film thickness, or heterogeneous nucleation, thereby initiating a complex dewetting process. The influence of intermolecular forces plays an important part in the rupture and in the subsequent dewetting process, where the formation of holes can be explained as the competition between the long-range attractive van der Waals and short-range Born repulsive intermolecular forces, which reduces the height of the unstable film to an even thinner layer of thickness ε that connects the evolving patterns and is closely related to the minimum of the corresponding intermolecular potential, i.e., the film settles into an energetically more favorable state. The early stages of this process are associated with the formation of regions of this minimal thickness, bounded by moving rims that connect to the undisturbed film and eventually destabilize.

Many studies have focused on the dynamics following rupture, such as the growing rim, or on the presence or vanishing of a damped oscillatory structure that joins the rim to the external undisturbed film. Concerning the latter problem, it was proposed that viscoelastic or shear thinning effects should play an important role. However, in a series of articles, see [1] and references therein, it was shown theoretically that the dynamics and morphology of the rims were due to the influence of interfacial slippage. In fact, the occurrence of interfacial slippage for liquid polymers has been discussed vividly in the literature, since it is of large technological interest, for example, to enhance the velocity of sliding fluid through microfluidic devices; see, e.g., [2] for a basic introduction. Moreover, also the formation of patterns in the wake of the destabilization of the rims depends on the occurrence of interfacial slippage [3].

The theoretical basis to understand this behavior is given by the thin film models that were derived in [1] over a wide range of slip lengths from the underlying equations for conservation of mass and momentum, together with boundary conditions for the tangential and normal stresses, as well as the kinematic condition at the free boundary, impermeability, and the so-called *Navier slip* condition at the liquid-solid interface. The derivation of these simplified models is based on the fact that the film thickness is much smaller than the typical length scales of the evolving patterns. As a result, one obtains dimension-reduced but high-order partial differential equations for the height h of the film

$$\partial_t h = -\partial_x \Big(M(h) \partial_x \left(\partial_{xx} h - \Pi(h) \right) \Big), \tag{1}$$

and

$$\mathrm{Re}\,(\partial_t u + u\partial_x u) = \frac{4}{h}\partial_x(h\partial_x u) + \partial_x\left(\partial_{xx}h - \Pi(h)\right) - \frac{u}{\beta h}, \tag{2a}$$

$$\partial_t h = -\partial_x\,(hu)\,, \tag{2b}$$

where $M(h) = h^3 + b\,h^2$, and $u(x,t)$ denotes the velocity of the film in the lateral direction. The slip-length parameters b and β are such that $b \ll \beta$. The terms $\mathrm{Re}\,(\partial_t u + u\partial_x u)$, with Re denoting the Reynolds number, represent the inertial forces, and $(4/h)\partial_x(h\,\partial_x u)$ the elongational viscosity of the moving liquid. The forces that actually drive the dewetting process are the intermolecular forces. The effective impact that these forces have on the surface of the film h can be approximated by

$$\Pi(h) = \frac{1}{\varepsilon}\left[\left(\frac{\epsilon}{h}\right)^3 - \left(\frac{\varepsilon}{h}\right)^4\right], \tag{3}$$

where $0 < \varepsilon \ll 1$ denotes the minimal thickness between the droplets.

While these models have shown tremendous success in describing the early and intermediate phases of the dewetting process, the description of the late phases, where large arrays of liquid droplets perform an intricate coarsening dynamics, is still a challenge.

Late-phase dynamics

The main property of interest here is the coarsening rate. However, even for simplified thin film models, the numerical simulations of the coarsening dynamics of large arrays of liquid droplets for sufficiently long times are far too time-consuming. The foundations to solve this problem were given by Glasner and Witelski [4], where under the assumption of a slow, near-equilibrium motion of the droplets, the thin film models have been simplified even further to systems of coupled ordinary differential equations describing the position X_k and pressure P_k of each droplet

$$\frac{dP_k}{dt} = C_P(P_k)\,(J_{k+1,k} - J_{k,k-1}), \quad \frac{dX_k}{dt} = -\,C_X(P_k)\,(J_{k+1,k} - J_{k,k-1})\,. \tag{4}$$

The dynamics is controlled by the fluxes between the droplets $J_{k+1,k}$, but also by the coefficients $C_P(P_k)$ and $C_X(P_k)$, which can be derived via asymptotic analysis from the thin film models. This has been done for the situation of no slip at the liquid-solid interface in [4]. Further extention to higher dimensions and mathematical analysis were undertaken in [5]. Our focus in [6] was the study of effects of slippage on the late-phase coarsening process, using the thin film model for large slippage (2a)–(2b). We derived similar systems of coupled ODEs, where now the coeffient $C_X(P_k)$ and the fluxes also depend on slippage.

The most interesting result in [6] shows that droplets not necessarily migrate in the direction opposite to the applied flux, as was established in [5] for the no-slip case. We can prove that there is a critical value of slippage $\beta = \beta_{cr}$ above which droplets migrate in the same direction as the flux. This fact can be explained by the impact of the new terms connected with the elongational viscosity that appears only in the thin film model for large slippage (2a)–(2b).

Proposition. *When ε and the pressure P of the droplet are sufficiently small, there exists a unique*

zero $\beta = \beta_{crit}(P, \varepsilon) << 1$ *of* $C_X(P_k)$ *as a function of* β, *which has the asymptotics*

$$\beta_{crit} = K\varepsilon \ln\left(\frac{2}{3\varepsilon P}\right) + o(\varepsilon), \tag{5}$$

such that the direction of the droplet migration is opposite (in the same direction as) the flux when $\beta < \beta_{crit}$ $(\beta > \beta_{crit})$.

This migration effect is illustrated in Figure 1. For a given array of three droplets, β_{crit} was calculated for the middle one, and then solutions of (4), (4) with three different values for the slip parameter $\beta_1 < \beta_2 = \beta_{crit} < \beta_3$ were obtained. Note that in the case $\beta = \beta_{crit}$, the middle droplet almost does not move. Moreover, we can show that the flux applied on the middle droplet is always negative. So in the case $\beta < \beta_{crit}$, it moves opposite to the flux, and in the case $\beta > \beta_{crit}$, in the same direction as the flux.

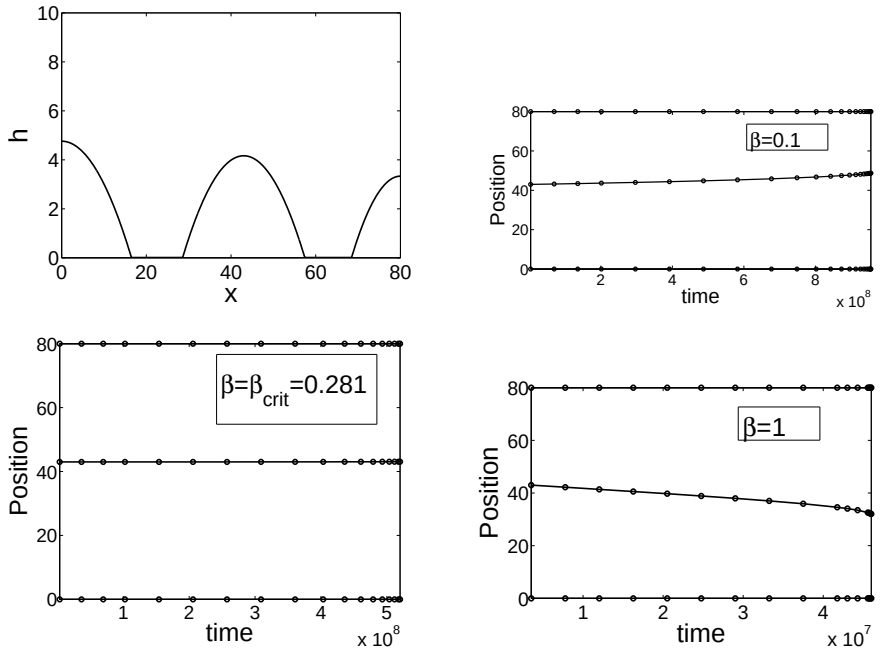


Fig. 1: *Migration of the middle droplet in the array of three droplets (upper left plot) for different* β. $L = 80$, $\epsilon = 0.01$, $Re = 0$, $P_2 = 0.4$

Coarsening behavior. It was shown in [7] that in contrast to the Cahn–Hilliard equation, used to describe coarsening processes, such as phase-separating binary alloys, the thin film models describing coarsening arrays of droplets demonstrate besides Ostwald ripening, i.e., droplet collapse, the existence of collisions of droplets as another coarsening mechanism. Our analysis demonstrates that this component may actually strongly influence the coarsening behavior when the slip length becomes large.

To illustrate some effects on the evolving pattern, we follow, as an example, the paths of eight droplets (black) in time in Figure 2, where we increase slippage, while keeping $\varepsilon = 0.1$ fixed.

We observe that the droplets tend to become less mobile at first and tend to coarsen via collapse (see middle row), but that if the slippage is further increased, droplets start to switch their direction

and increase their mobility, and that eventually the coarsening behavior is dominated by collisions (bottom row). As a consequence, this has considerable impact on the coarsening rates.

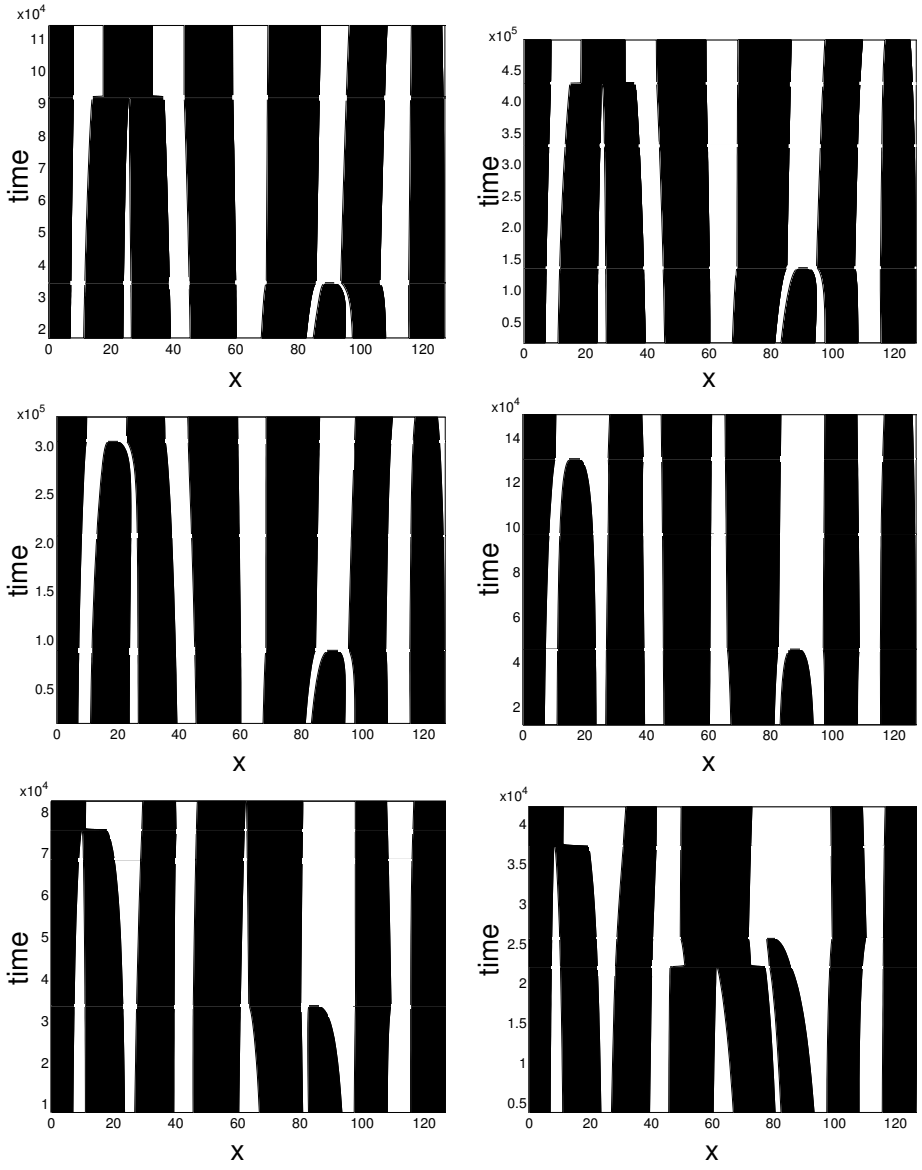


Fig. 2: *First two coarsening events in the initial array for six different slip values: Intermediate slip, large slip model with* $\beta = 0.3$, $\beta = 0.5$, $\beta = 1.25$, $\beta = 2$, $\beta = 3.5$ *(arranged from left to right and from top to bottom)*

Coarsening rates. The value of the slip-length parameter β large slip considerably influences the coarsening behavior of an initial system of droplets and the contribution of the collision component, depending on how close this value is to the mean critical slip length of the system. We found that this fact implies a dependence of the collision-dominated coarsening rates on the value of the slip length.

In [4], the coarsening dynamics of initially well-separated systems of droplets was investigated, which experience in general only collapse coarsening effects (so-called *collapse-dominated coars-*

ening rates), and it was shown that the statistical number of droplets $N(t)$ in such a system changes in time according to

$$N(t) \propto t^{-2/5}. \tag{6}$$

In another publication, the lubrication model (1) was considered with mobility term $M(h) = h$, and the law (6) was derived on the basis of the gradient flow structure of the equation. As the equation for the evolution of droplet pressures is the same in the reduced models for all slip regimes, it is natural to expect that the coarsening-rate law for collapse-dominated systems does not depend on the chosen slip regime and is always given by (6). Moreover, in [7] it was shown that for the one-dimensional no-slip regime, any initial system of droplets will coarsen, according to (6) independently of the proportional number of collision and collapse events during the coarsening process.

We simulated for various initial configurations and numbers of points N the coarsening dynamics of the intermediate-slip regime and found (as was expected from the results of [5]) that the percentage of collisions is very small. As is claimed in [5], the intermediate-slip regime is essentially collapse dominated and, hence, coarsening rates for it are given by (6).

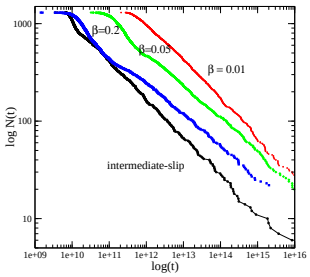


Fig. 3: *Coarsening rates for intermediate to large slip with $\beta = 0.2$, $\beta = 0.05$, and $\beta = 0.01$*

We then solved the reduced system (4) for the corresponding strong-slip model for similar initial distributions of droplets and values for the slip-length parameters $\beta = 0.2$, $\beta = 0.05$, and $\beta = 0.01$. We observed firstly that the proportion of collisions became dominant and increased with slippage. Secondly, the corresponding coarsening rates had slopes $\sim t^{-1/3}$ for $\beta = 0.2$ and decreased to $\sim t^{-2/5}$, as shown in Figure 3.

The analytical derivation and more precise analysis for the dependence of collision-dominated coarsening rates on the slip length in the strong-slip regime is subject of our ongoing research.

References

[1] A. Münch, B. Wagner, T.P. Witelski, *Lubrication models with small to large slip lengths*, J. Engr. Math., **53** (2006), pp. 359–383.

[2] P.G. de Gennes, *Wetting: Statics and dynamics*, Rev. Mod. Phys., **57(3)** (1985), pp. 827–863.

[3] J.R. King, A. Münch, B. Wagner, *Linear stability of a ridge*, Nonlinearity, **9** (2006), pp. 2813–2831.

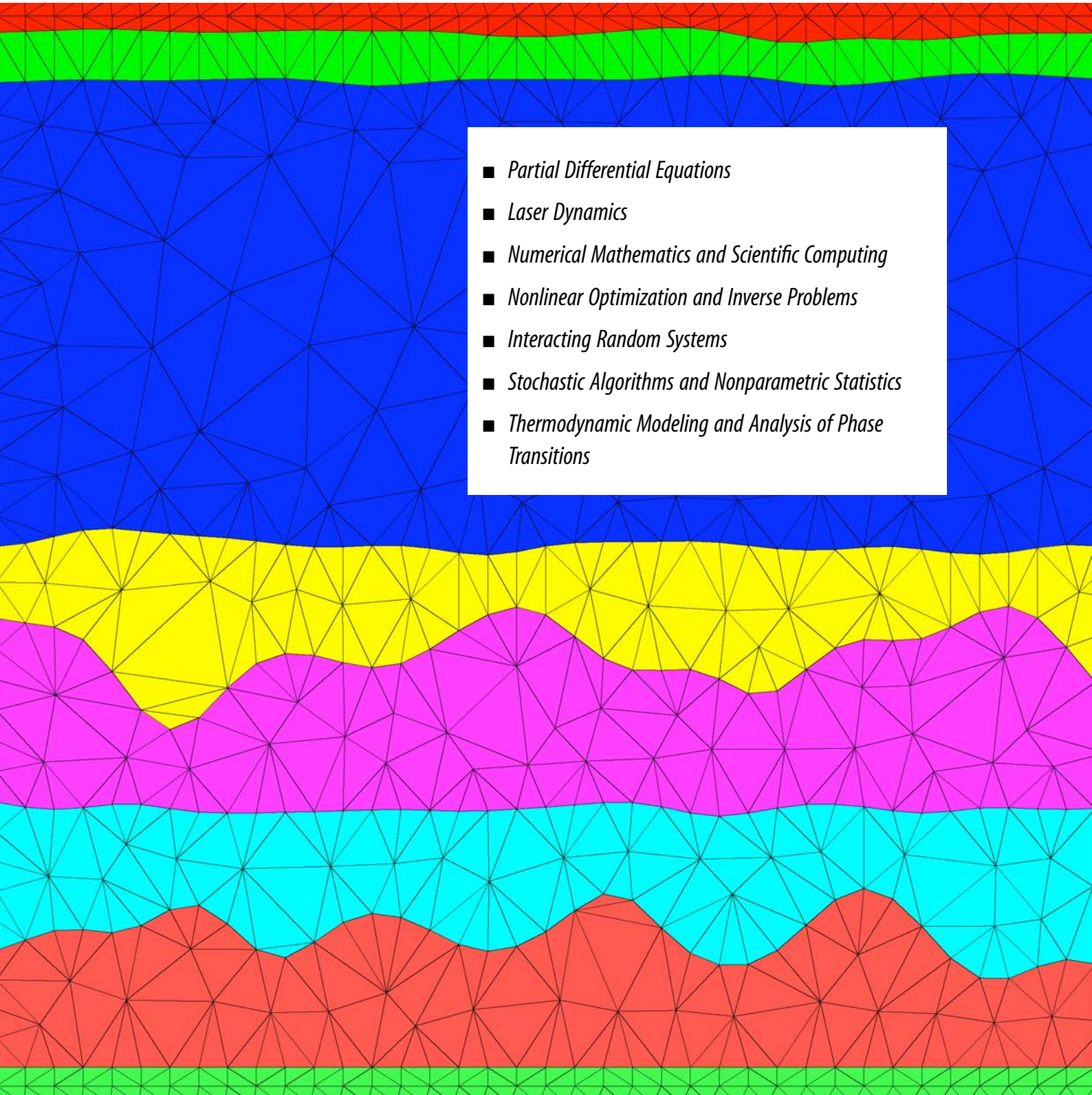
[4] K.B. Glasner, T.P. Witelski, *Coarsening dynamics of dewetting films*, Phys. Rev. E, **67** (2003), pp. 016302/1–016302/12.

[5] K. Glasner, F. Otto, T. Rump, D. Slepčev, *Ostwald ripening of droplets: The role of migration*, Europ. J. Appl. Math., **20(1)** (2009), pp. 1–67.

[6] G. Kitavtsev, B. Wagner, *Coarsening dynamics of slipping droplets*, WIAS Preprint no. 1381, 2008, submitted.

[7] K.B. Glasner, T.P. Witelski, *Collision vs. collapse of droplets in coarsening of dewetting thin films*, Phys. D, **209** (2005), pp. 80–104.

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 1 *Partial Differential Equations*

The main focus of this research group is the analytical understanding of partial differential equations, which is essential for the modeling of problems in the sciences and engineering. The theory is developed in close connection with well-chosen problems in applications, mainly in the following areas:

- Evolutionary systems with applications in material modeling and in semiconductor devices
- Modeling of optoelectronic devices including quantum effects
- Multifunctional materials and plasticity

The mathematical methods range from pure functional analysis and mathematical physics to modeling and numerical methods:

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

The study of the well-posedness of the partial differential equations leads to a deeper understanding of the underlying physics and provides a basis 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 the optimization of technological products.

Material Modeling

MICROPLAST

Fig. 1: *Research Unit 797 (supported by DFG)*

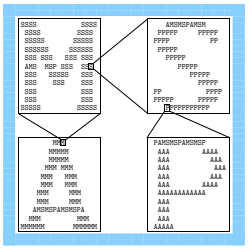
Research in the area of material modeling was devoted to viscous models and to rate-independent models. The DFG Research Unit FOR 797 "Analysis and computation of microstructure in finite plasticity" involves mathematical and engineering groups in Berlin, Bochum, Bonn, Düsseldorf, Leipzig, Regensburg, and Stuttgart. At WIAS, the subproject P5 "Regularizations and relaxations of time-continuous problems in plasticity" started in April 2008 with the employment of Sebastian Heinz, who finished his Ph.D. studies in July with the thesis entitled "Preservation of quasiconvexity and quasimonotonicity in polynomial approximation of variational problems". A first existence result for elastoplastic processes at finite strain, which are based on the multiplicative decomposition of the strains, was obtained and presented at the international engineering conferences (IUTAM) in Cape Town and Bochum.

The MATHEON project C18 "Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys" investigates isothermal as well as temperature-driven models for phase transformations in shape-memory materials that are suited for a mathematical

treatment, giving existence, uniqueness, and numerical approximation results. Moreover, elastodynamical contact problems for viscous materials have been studied; see [3]. Florian Schmid investigated finite-dimensional, quasistatic contact mechanics with Coulomb friction, giving a first rigorous theory for curved boundaries. In his Ph.D. thesis entitled "Analysis of geometrically nonlinear models for contact with dry friction" (defended in July 2008) he carefully investigated the influence of the boundary geometry on the existence of solutions. He also initiated a seminar for all doctoral students employed at WIAS.

Fig. 2: *Illustration of the influence of curvature in geometrically nonlinear contact problems*

In the year 2008, the DFG Priority Program SPP 1095 "Analysis, Modeling and Simulation of Multiscale Problems", which was coordinated by Alexander Mielke, came to its official end. The WIAS project "Macroscopic dynamics in discrete lattices" investigated the infinite-dimensional dynamics in Hamiltonian lattice models. In particular, the question of upscaling discrete microscopic models to continuous macroscopic models was studied; see [1]. The aspects of dispersive decay of initial disturbances in an infinite lattice were investigated by studying the important question as to which nonlinearities are strong enough to counterbalance the linear dispersive decay. Figure 3 displays a simulation for the square lattice $\mathbb{Z}^2$ with nearest-neighbor interaction, where the initial disturbance is given at $(300, 0)$.



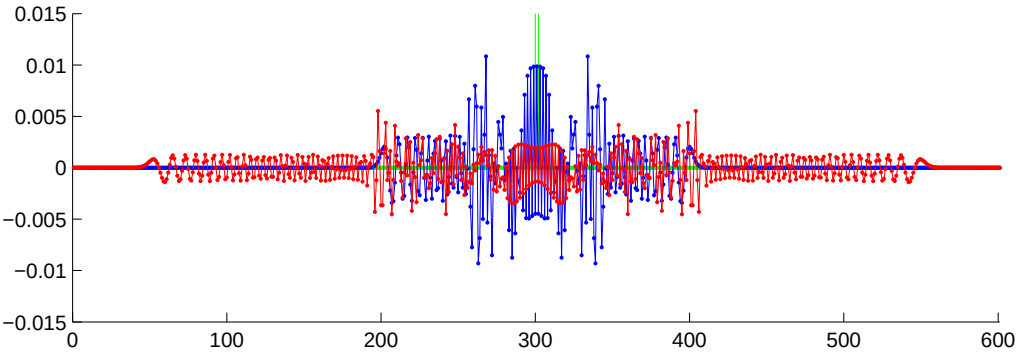


Fig. 3: *Displacements of lattice points $(j, 0)$ for $j = 0, \ldots, 600$ at the times $t = 5$ (green), $t = 100$ (blue), and $t = 250$ (red)*

A series of papers was also devoted to damage and crack evolution in elastic materials. Previous work on cracks was extended from the small-strain case to geometrically nonlinear elastic materials. Assuming that the crack path is known in advance, a local, rate-independent model was developed on the basis of Griffith's fracture criterion. Due to the nonuniqueness of the minimizing deformations, the reduced elastic energy is no longer differentiable with respect to the time and to the position of the crack tip. Thus, the fracture evolution has to be formulated using a generalized subdifferential extending the classical crack evolution models for elasticity with strictly convex energies to the finite strain case; see [2].

Fig. 4: *Interdisciplinary Centre for Mathematical and Computational Modelling, Warsaw*

The Workshop on Free Boundaries and Materials Modeling took place at WIAS from March 17 to 18, 2008, and was organized by Dorothee Knees, Christiane Kraus, and Alexander Mielke. The idea was to bring together the interested scientists from the DFG Research Center MATHEON, the Interdisciplinary Centre for Mathematical and Computational Modelling (ICM) Warsaw, and WIAS. Analytical and mechanical models for multifunctional materials such as semiconductors, shape memory alloys, lithium batteries, and ferromagnets were discussed.

The grant proposal "Modeling of damage processes", which was submitted by Dorothee Knees and Christiane Kraus (Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*) in the framework of the competition "Pakt für Forschung und Innovation" of the German Leibniz Association, has been approved. This grant provides the funding for a new subgroup at WIAS (called *Leibniz Group 2*) starting in January 2009. The goal of the project is to derive and analyze reliable models for the description of damage and failure.

Regularity theory for partial differential equations

Regularity properties for solutions of partial differential equations were investigated from a quite general perspective. Intrinsic problems arise in models of materials where the properties change abruptly at interfaces, so-called *heterostructures*, which are common in semiconductor devices. Using conceptually new methods like Gaussian estimates, it was possible to generalize results that are well known in the smooth case; [7]. A substantially new aspect is the application of the obtained regularity properties of the solution in optimal control of PDEs, which is joint research with the Research Group *Nonlinear Optimization and Inverse Problems*.

The investigation of spatial regularity for elastoplastic models was continued as well. Using a reflection argument, a global spatial regularity result for the displacements, stresses, and internal variables was proved for rate-independent elastoplasticity with linear hardening.

Semiconductor modeling

Fig. 5: *Participants of the MesoTrans 2008*

The Fourth Workshop on Mathematical Models for Transport in Macroscopic and Mesoscopic Systems (MesoTrans 2008) took place at WIAS from February 7 to 10, 2008, and was organized by

Hagen Neidhardt, Paul Racec, and Joachim Rehberg. The topics discussed involved the modeling of charge transport in semiconductor devices using ideas from non-equilibrium steady state theory on the one hand and mesoscopic models for semiconductors on the other hand.

In semiconductor devices on the nanoscale, the functionality depends on effects that have to be described via quantum mechanics. In this field, a closed theory for the nanowire transistor was developed; see the Scientific Highlights article on page 20. In the MATHEON project D4 "Quantum mechanical and macroscopic models for optoelectronic devices", new structural insights in the Kohn–Sham system from Density Functional Theory were found, including the analytic dependence of the particle density on the Schrödinger potential; see [4]. Based on these ideas, it was possible to derive new and stable numerical algorithms for calculating the quantum-mechanical properties of nanoelectronic devices. Moreover, a solution theory for a Kohn–Sham system at zero temperature has been achieved [5].

Modern spintronic semiconductor devices are described by additional particles leading to so-called *spin-polarized drift-diffusion models*. These systems were first analyzed with respect to existence and uniqueness results and to suitable a priori bounds for the time-dependent problem. For the case that the boundary data are compatible with the thermodynamic equilibrium, it was shown that the free energy along the solution decays monotonously and exponentially to its equilibrium value. In further work in cooperation with the Research Group *Numerical Mathematics and Scientific Computing*, the existence and uniqueness of steady states were obtained, even under Dirichlet boundary conditions that are only nearly compatible with the thermodynamic equilibrium. The same properties were obtained for a space-discretized version of the problem, namely the Scharfetter–Gummel scheme on three-dimensional boundary-conforming Delaunay grids. Also for electro-reaction-diffusion systems, a discretization scheme in space and time was established that preserves the main features of the corresponding continuous problem, namely positivity, dissipativity, and the monotone and exponential decay of the free energy to its equilibrium value [6].

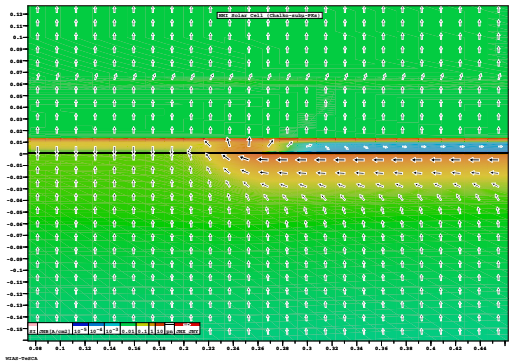


Fig. 6: *Electron current through a structured passivation layer inside a thin-film solar cell based on wider band-gap chalcopyrites*

In the area of photovoltaics, the Research Groups *Partial Differential Equations* and *Numerical Mathematics and Scientific Computing* started to cooperate with the relevant groups in the Helmholtz Centre Berlin for Materials and Energy. Most designs of present-day solar cells are based on one-dimensional simulations. However, novel concepts like rough interfaces or new geometries for the electric contact rely on multidimensional effects. Two- and three-dimensional simulations in thin-film solar cells were performed by using the software tool `WIAS-TeSCA`. It was possible to

make systematic parameter studies in terms of the point-contact radius and the interfacial defect density of states. Thus, it was confirmed that the equipment of a standard device with electrically conducting point contacts embedded in an appropriate passivation layer is beneficial for the performance of solar cells.

References

[1] J. Giannoulis, M. Herrmann, A. Mielke, *Lagrangian and Hamiltonian two-scale reduction*, J. Math. Physics, **49(19)** (2008), pp. 103505/1–103505/42.

[2] D. Knees, C. Zanini, A. Mielke, *Crack growth in polyconvex materials*, WIAS Preprint no. 1351, 2008, to appear in: Phys. D.

[3] A. Petrov, M. Schatzman, *Mathematical results on existence for viscoelastodynamic problems with unilateral constraints*, WIAS Preprint no. 1216, 2007, to appear in: SIAM J. Math. Anal.

[4] K. Hoke, H.-Chr. Kaiser, J. Rehberg, *Analyticity for some operator functions from statistical quantum mechanics*, WIAS Preprint no. 1373, 2008, submitted.

[5] H. Cornean, K. Hoke, H. Neidhardt, P.N. Racec, J. Rehberg, *A Kohn–Sham system at zero temperature*, J. Phys. A, **41** (2008), pp. 385304/1–385304/21.

[6] A. Glitzky, *Exponential decay of the free energy for discretized electro-reaction-diffusion systems*, Nonlinearity, **21** (2008), pp. 1989–2009.

[7] M. Hieber, J. Rehberg, *Quasilinear parabolic systems with mixed boundary conditions*, SIAM J. Math. Anal., **40(1)** (2008), pp. 292–305.

3.2 Research Group 2 *Laser Dynamics*

The research of this group is devoted to the development of mathematical methods and theories in the field of nonlinear dynamics, with applications in optoelectronics. The main topics in 2008 were *dynamics of semiconductor lasers* and *pulses in nonlinear optical media*. The research related to these topics includes mathematical modeling, theoretical research on dynamical systems occurring in laser theory and nonlinear optics, numerical implementation, and device simulation.

An important event in the previous year was the International Workshop *"Complex Dynamics in Large Coupled Systems"*, November 17 – 19, organized together with colleagues from the Free University (FU) of Berlin, the Humboldt University (HU) of Berlin and the Forschungszentrum (research center) Jülich. The aim of the workshop was to discuss recent developments in the field of complex dynamics in coupled systems, related not only to theory but also to applications in optoelectronics and neuroscience.

The group has extended their teaching activities through a special lecture at HU Berlin, in addition to their two traditional research seminars "Mathematical Photonics" and "Nonlinear Dynamics", organized together with HU and FU Berlin, respectively.

Again, Uwe Bandelow was a member of the Program Committee of NUSOD for its 2008 conference in Nottingham, UK.

In the framework of the new DFG Collaborative Research Center (SFB) 787 "Semiconductor Nanophotonics: Materials, Models, Devices", the group started two projects:

1. B4: "Multi-dimensional modeling and simulation of VCSEL devices" (jointly with Alexander Mielke, Research Group *Partial Differential Equations*, and Frank Schmidt, Zuse Institute Berlin). The activities concentrated on the mathematical modeling, especially on the efficient coupling of the optical with the electrical model, and with respect to the latter, on the inclusion of quantum structures into the spatially resolved transport model.
2. B5: "Effective models, simulation, and analysis of the dynamics in quantum dot devices" (jointly with Jürgen Sprekels, Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*). Here, an efficient numerical scheme for modeling dynamical instabilities in monolithic passively mode-locked semiconductor lasers was proposed that is based on the integration along the characteristics of the traveling wave equations describing the space-time evolution of counter-propagating waves in those lasers. This scheme was used to describe typical bifurcation sequences that occur with the increase of the injection current in the laser gain section.

Furthermore, the progress in the following fields of research should be mentioned:

Numerical methods for laser dynamics

Based on the spatially extended large-scale traveling wave model for the dynamics of broad-area semiconductor lasers, theoretical investigations for master-oscillator-power-amplifier devices have been performed with good results. Simulation results have been compared with experimental data obtained at the Ferdinand Braun Institute for High Frequency Technology (FBH), Berlin,

and are shown in joint publications [1]. Different numerical algorithms for high performance parallel computations have been discussed [2]. These algorithms have been successfully implemented and tested on the new WIAS Euler compute cluster. A simulation tool has been obtained, which is used for further investigations of different high-brightness semiconductor laser device concepts.

Dynamics of laser systems with delayed coupling or feedback

In 2008, the group's software `LDSL-tool` has been used to study the following different semiconductor lasers and coupled laser systems:

1. Wavelength stabilization of Fabry–Perot lasers by external volume Bragg gratings: This work was done under contract with FBH, Berlin.
2. Simulation and analysis of semiconductor ring lasers: In order to model the ring lasers, the traveling wave model and the software `LDSL-tool` have been properly extended. These modifications allow to consider various self- and cross-gain saturations, as well as asymmetric detuning and field losses for different counterpropagating fields.

Chaos communication has been the topic of a cooperation with the University of the Balearic Islands (Palma, Spain). Results of numerical investigations of the dynamical behavior of a single-mode semiconductor laser under the influence of multi-cavity optical feedback have been reported in [3]. Under certain conditions, the system was found to display chaotic behavior, appropriate for chaos-based communications. The synchronization of two unidirectional coupled (master-slave) systems has also been studied. Very good conditions for message encoding by using chaos modulation and on/off phase shift keying encryption methods have been identified. Examples of message encoding/decoding have been presented.

Within the DFG Collaborative Research Center SFB 555 "Complex Nonlinear Processes", the research on coupled laser systems has been continued with a special emphasis on stability properties in large coupled systems and systems with long-delayed feedback [4].

Pulses in nonlinear optical media

The formation and properties of localized solitary structures propagating in nonlinear media, placing special emphasis on the behavior of ultrashort optical pulses in fused silica, were considered both numerically and theoretically in the projects D14 "Nonlocal and nonlinear effects in fiber optics" and D20 "Pulse shaping in photonic crystal fibers" of the DFG Research Center MATHEON "Mathematics for key technologies".

A local dispersion operator, which is de facto used by most envelope equations, cannot completely quantify dispersion for ultrashort optical pulses [5]. Therefore, a nonlocal pseudodifferential dispersion operator was introduced that yields an adequate description of arbitrary medium dispersion and absorption in a wide spectral region. On this basis, both envelope and non-envelope models for pulse propagation were formulated and investigated. These models correctly describe the dynamics of few-cycle and even sub-cycle optical pulses.

In the DFG project "Pulse shaping in hollow-fiber compressors: Simulation and experiment", which includes experiments at the Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin, filamentary self-compression has been investigated. Filamentary propagation of ultrashort pulses in gases is basically a free-space propagation scenario. It has been demonstrated that the recently observed filamentary self-compression is dominated by spatial effects. Based on a variational approach, analytical models for both the pulse breakup in the first plasma-dominated regime and the subsequent Kerr-dominated regime have been presented. These models successfully reveal the origins of filamentary self-compression.

Dynamical systems

It is common in semi-arid or arid regions to encounter landscapes where the vegetation cover is non-uniform and exhibits large-scale structures, usually referred to as *vegetation patterns*. In [6], a mathematical model describing the formation of vegetation patterns and localized bare soil spots (sometimes also called *fairy circles*) in arid vegetation ecosystems has been presented. Interactions of localized bare spots have been studied both analytically and numerically. When the distance between them is large, bare spots do not interact. They form an isolated stationary structure. However, if they are located close to each other, they start to interact through their overlapping tails. The interaction forces the bare spots to move until they reach a stable equilibrium position. It was shown that there exist several equilibrium positions [6]. The system selects one of these positions, depending on the initial distance between the two localized spots.

References

[1] M. Spreemann, M. Lichtner, M. Radziunas, U. Bandelow, H. Wenzel, *Measurement and simulation of distributed-feedback tapered master-oscillator power amplifiers*, to appear in: IEEE J. Quantum Electron.

[2] R. Ciegis, M. Radziunas, M. Lichtner, *Numerical algorithms for simulation of multisection lasers by using traveling wave model*, Math. Model. Anal., **13** (2008), pp. 327-348

[3] V.Z. Tronciu, C.R. Mirasso, P. Colet, *Chaos-based communications using semiconductor lasers subject to feedback from an integrated double cavity*, J. Phys. B: At. Mol. Opt. Phys., **41** (2008), pp. 155401/1–155401/8. Also in: Collected Articles from the Institute of Physics. IoP Select 2008–2009.

[4] S. Yanchuk, M. Wolfrum, *Destabilization patterns in large regular networks*, Phys. Rev. E, **77** (2008), pp. 026212/1–026212/7.

[5] S. Amiranashvili, A.G. Vladimirov, U. Bandelow, *Solitary-wave solutions for few-cycle optical pulses*, Phys. Rev. A, **77** (2008), pp. 063821/1–063821/7. Also in: Virtual J. Ultrafast Sci., 2008.

[6] M. Tlidi, R. Lefever, A.G. Vladimirov, *On vegetation clustering, localized bare soil spots and fairy circles*, in: Dissipative Solitons: From Optics to Biology and Medicine, N. Akhmediev, A. Ankiewicz, eds., vol. 751 of Lect. Notes Phys., Springer, Berlin/Heidelberg, 2008, pp. 381–402.

3.3 Research Group 3 *Numerical Mathematics and Scientific Computing*

The mathematical description of many 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. Numerical methods can be applied to calculate approximate solutions.

Systems of differential–algebraic equations (DAE), i.e., of ordinary differential equations and additional algebraic equations, are used in situations where the spatial structure of the problem is not present or can be ignored. Among many other problems, electrical networks and processes in chemical plants can be modeled by this type of description.

Partial differential equations (PDEs) are used to model problems where the spatial structure of the model has to be taken into consideration. The unknowns in PDEs are functions of one or several spatial variables and, possibly, of time. Within the large class of problems of this type, the group focuses on applications in the fields of semiconductor device modeling, electrochemistry (see the Scientific Highlights article on page 49) and porous media flow.

Differential equations and their solutions are represented on the computer in an approximate way, using finite-dimensional models created by discretization in time and space. After this discretization step, one is left with a large system of linear (or nonlinear) equations that needs to be solved in an efficient and accurate way. Specific for the discretization of partial differential equations is the process of mesh generation, i.e., the subdivision of the computational domain into a finite number of polygonal elements, which then allow to create finite element or finite volume approximations. Finally, in order to be useful, the implementation of these methods into software is essential, including the possibility to visualize results. In what follows, current activities of the group in several of the described fields are listed.

Numerical solution of large DAE systems

The group develops and maintains the block-oriented process simulator `BOP`. This simulator is based on a divide-and-conquer method. Currently, the main application field is the simulation of gas turbines in cooperation with ALSTOM Power Ltd. In 2008, version `BOP2.4` has been delivered to the partner. This version provides four different simulation modes: steady state, transient, Monte Carlo, and correction curves, and is used now for process development as well. A long-term cooperation and support agreement between ALSTOM Power Ltd. and WIAS has been signed.

Version `BOP2.5` is in progress, and will be delivered in 2009. Its user interface will be based on the new process modeling language MLBOP whose functionality is comparable to that of the standard process modeling language for industrial process simulation. A compiler has been developed that creates the simulation code from the process model described in MLBOP. A converter between the industry-standard language and MLBOP is under development. Different possibilities for process optimization are investigated with the aim to enhance the functionality of future `BOP` versions by optimization methods.

Mesh generation

The group focuses on algorithms for the generation of three-dimensional boundary-conforming Delaunay meshes that are necessary for the implementation of the Voronoi box based finite volume method [6], [7]. The mesh generator TetGen developed in this project is established on the international level. A number of cooperation and license requests created options for future collaborations.

A new method for the validation and storage of three-dimensional polyhedra was developed [8], which was funded by the Dutch research network Ruimte voor Geo-Informatie, in cooperation with the Delft University of Technology (Research Institute OTB, section GISt), and based on TetGen's technology.

Fig. 1: *A view of a tetrahedral mesh generated by TetGen*

Software environment for the numerical solution of partial differential equations

The software environment `pdelib2` provides a framework to integrate the different stages of numerical algorithm development, including mesh generation, numerical solution, and visualization. It is used in a number of projects within WIAS, e.g., laser hardening of steel, electrochemical modeling, and post exposure bake in photolithography. In 2008, work on the core functionality focused on the development of new structures for finite element computations, for optimal control, and for B-splines. A new, more versatile sparse matrix class has been introduced, and grid partitioning for parallel computations has been improved. The overall code structure has been modularized; resource directories allow the users to relocate binaries. New methods for persistent data and configuration storage, GUI creation, and macro recording, as well as ports to new compilers make the code more flexible with respect to its use in applied projects. Visualization capabilities have been improved by the inclusion of particle tracking and the possibility to create stereo and multi-view projections.

Three-dimensional semiconductor device simulation

The group successfully concluded a three-year research contract for improving the simulation basis for detectors in high energy and astrophysics with the European XFEL GmbH, the company operating the future X-ray free electron laser to be constructed in Hamburg. Special questions regarding the design of detectors for huge clouds of electron-hole pairs have to be considered in collaboration with groups at Hamburg University, the Rutherford Appleton Laboratory (Oxfordshire), and the Max-Planck-Institut Halbleiterlabor (semiconductor laboratory) in Munich. The first measurements done by J. Becker at the Institute for Experimental Physics, University of Hamburg, using short-pulse laser illumination with different spot sizes, generated large carrier numbers. The experiments are based on GHz oscilloscopy and are now recomputed using nonlinear mobility models.

The correction of the computed data by modeling secondary effects, such as parasitic capacitances, coaxial cables of known length, preamplifier, etc., in the measurement setup will be the next step towards direct comparison.

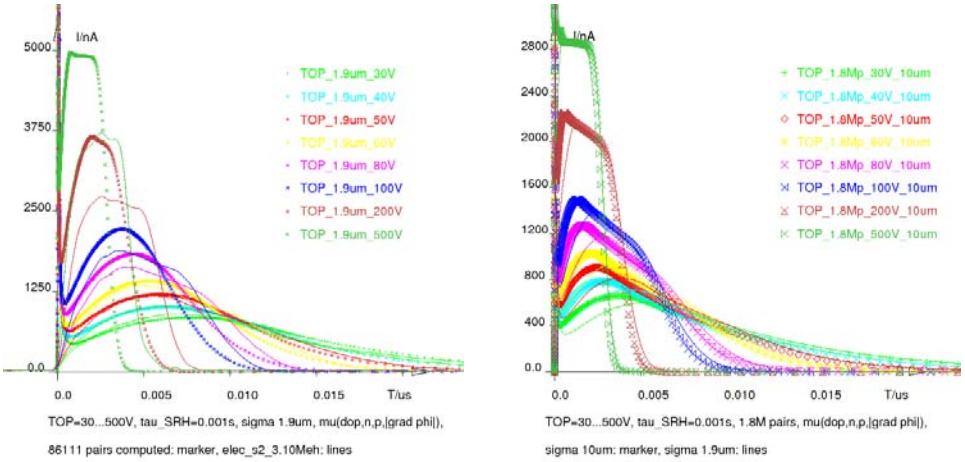


Fig. 2: *Comparison of computations and measurements (left) and the influence of the initial density (variation 1 : 25; marker: lines) of the charge cloud—the largest influence of the nonlinearities is expected at small times (right)*

Figure 2 shows computed and measured data for different applied voltages (depletion is reached in computations close to 60 V, 86,111 electrons and holes are created close to the bottom and the center of a 10-degree sector of a pin diode or 3.1 million pairs in the experiment). The region below a few nanoseconds cannot be resolved by the measurements directly.

Within the framework of the DFG Collaborative Research Center SFB 787 (see also page 16), the group collaborates with the Research Groups *Partial Differential Equations* and *Laser Dynamics*, the Technical University of Berlin, and the Zuse Institute Berlin on the three-dimensional modeling of vertical-cavity surface-emitting lasers (VCSEL). Current work focuses on a new model of the main effects of quantum-dot-stimulated emission and absorption processes, including a quantum-well wetting layer that shall be coupled to the drift-diffusion approximation and the optical properties of the cavity. Tests with respect to III-V semiconductors will follow soon.

Simplified three-dimensional mode selection studies with broken cylindrical symmetry by electrical contacts and the relatively small confinement in the vertical direction illustrate the complexity of the problem (compare Figure 3).

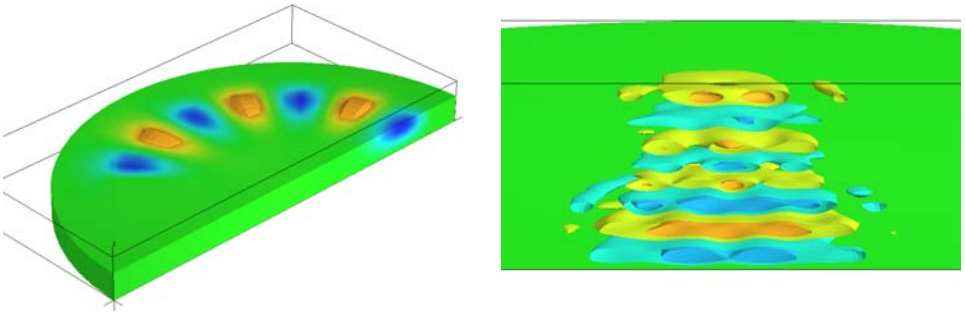


Fig. 3: *Symmetry breaking due to contacts, the contact at the left end of the 180-degree arc suppresses oscillations, 13th eigenfunction (left). The eigenvector close to the desired 4 λ case is neither rotationally symmetric nor fits into the numerical approximation of the cavity (right)*

The work aiming at an improved theoretical foundation was continued. Main results have been, for instance, analytical and discrete existence proofs [5]. The work at WIAS over many years was honored by an invitation to give a talk at the Pixel 2008 Workshop at the Fermi National Accelerator Laboratory in Batavia, Illinois.

Post exposure bake in photolithography

Photolithography is an essential step during the manufacturing of semiconductor devices. It consists of 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*: At an increased temperature, chemical reactions transform an acid distribution created by the light into a distribution of a dissolution inhibitor that resists the later applied etching agent.

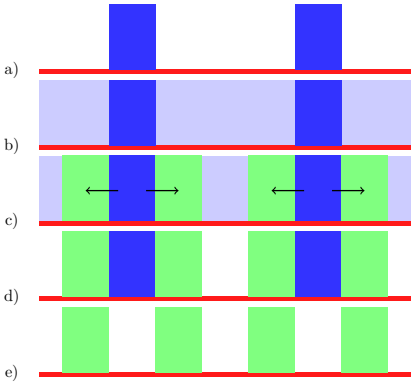


Fig. 4: *Schematic of pattern doubling process steps. A primary structure, containing a deposit of acid (a), is overcoated by a new spacer (b). A certain amount of residual acid leaves the primary structure by diffusion, initiating cross-linking of the spacer, its spread being controlled by a certain amount of base added (c). Non-cross-linked material is developed (d) and etched away together with the original pattern (e)*

WIAS takes part in the Specific Targeted Research Project MD^3 "Material Development for Double Patterning and Double Exposure" funded by the European Commission within its 7th framework program. This research network is aimed at the development of strategies for the creation of 32 nm structures using current optical techniques.

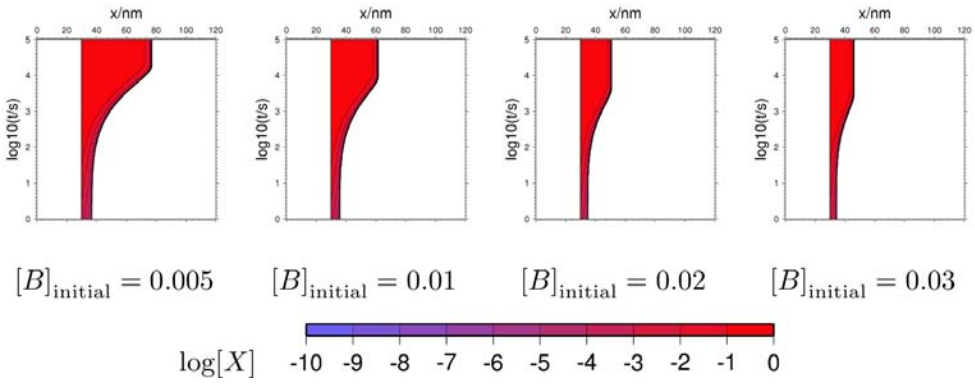


Fig. 5: *Simulated space-time plots of the spread of cross-linked material for different initial concentrations of a base added to control the process*

Based on a module for the solution of time-dependent reaction-diffusion problems on general geometries, which enables a flexible definition of reaction and diffusion models to describe various phenomena occurring during the post exposure bake and allows computations on general domains, a post exposure bake module has been integrated into the lithography simulation toolbox "Dr. LiTHO" of the project partner Fraunhofer Institute of Integrated Systems and Device Technology (IISB), Erlangen.

In cooperation with the project partners from Fraunhofer IISB, Erlangen, and Rohm & Haas Electronic Materials, Marlboro, Massachusetts, a prototypical reaction-diffusion model of cross-linking of a spacer catalyzed by acid diffusing out of a primary structure has been developed [3]. A schematic of the process is depicted in Figure 4. Simulation results are shown in Figure 5.

Leibniz Group 1 *Coupled flow processes in energy and environmental research*

The efficient and accurate simulation of coupled flow processes is an important and in many cases not yet satisfactorily solved problem in many applications in fields like energy, climate, geological and environmental research. In the framework of the competitive procedure of the Leibniz Association, the group successfully applied for the funding of a research network joining WIAS, the Free University of Berlin, the Potsdam Institute for Climate Impact Research, and the University of Erlangen. The network focuses on coupled flow processes in electrochemical systems like fuel cells and on the coupling between flow processes in the atmosphere and in the soil. In 2008, the Leibniz Group 1 has been formed at WIAS in order to bundle the resources allocated to this project.

Starting from the experience gathered for the mass conservative coupling of incompressible fluid flow and species transport [4], based on the use of the pointwise divergence-free finite element method [1] coupled to the Voronoi box based finite volume method, current work at WIAS focuses on the development of finite volume methods for the discretization of fluid flow with discrete mass conservation properties. The problem of coupling numerical models of free flow and porous media flow arises in a number of application problems. A deeper understanding of the choice of the interface condition is aimed at the development of a mass conservative finite volume method for the numerical approximation of this problem [2].

References

[1] E. Burman, A. Linke, *Stabilized finite element schemes for incompressible flow using Scott–Vogelius elements*, Appl. Numer. Math., **58** (2008), pp. 1704–1719.

[2] M. Ehrhardt, J. Fuhrmann, A. Linke, E. Holzbecher, *Mathematical modeling of channel-porous layer interfaces in PEM fuel cells*, in: Fundamentals and Developments of Fuel Cells, B. Davat, D. Hissel, eds., Proceedings of the Conference on Fundamentals and Development of Fuel Cells, University of Nancy, Dec. 10–12, 2008. ISBN 978-2-7466-0413-1.

[3] J. Fuhrmann, A. Fiebach, M. Uhle, A. Erdmann, C. Szmanda, C. Truong, *A model of self-limiting residual acid diffusion for pattern doubling*, to appear in: Microel. Engrg., Proceedings of the Micro- and Nano-Engineering 2008 Conference — MNE 2008.

[4] J. Fuhrmann, A. Linke, H. Langmach, H. Baltruschat, *Numerical calculation of the limiting current for a cylindrical thin layer flow cell*, submitted.

[5] A. Glitzky, K. Gärtner, *Existence of bounded steady state solutions to spin-polarized drift-diffusion systems*, WIAS Preprint no. 1357, 2008, submitted.

[6] H. Si, K. Gärtner, *Boundary recovery by constrained Delaunay tetrahedralization*, submitted.

[7] H. Si, K. Gärtner, J. Fuhrmann, *Boundary conforming Delaunay mesh generation*, submitted.

[8] E. Verbree, H. Si, *Validation and storage of polyhedra through constrained Delaunay tetrahedralizations*, in: Geographic Information Science, M.J. Egenhofer, D.M. Mark, eds., vol. 2478 of Lecture Notes in Computer Science, Springer, Berlin, 2008, pp. 354–369.

3.4 Research Group 4 *Nonlinear Optimization and Inverse Problems*

The research group investigates large-scale optimization and inverse problems occurring in current engineering and economic applications. The tasks range from basic research on analysis and numerics to the development of efficient algorithms and software to the solution of real-world problems.

Part of the research is carried out within the projects C7, C11, and C21 of the DFG Research Center MATHEON and within two projects in the DFG Priority Programs SPP 1180 and SPP 1204, respectively (see page 97). The group takes part in the Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", supervising two Ph.D. projects. Another Ph.D. thesis is supervised in the framework of a double doctorate project between the Technical University of Berlin and the Scuola Normale Superiore in Pisa.

In 2008, the group has further extended its successful collaboration with industry and partners from the engineering sciences. In the field of optimization problems under probabilistic constraints, a previously initiated collaboration with the research department of Electricité de France (EDF) led to a funded project aiming at new approaches to the control of hydraulic power units.

Another highlight is a new collaboration in the field of conical diffraction, i.e., the scattering of plane waves by multicoated diffraction gratings in the case of oblique incidence. Its integral formulation proposed in [8] leads to a system of singular integral equations over the nonsmooth grating profiles. For the case of non-coated gratings, algorithms have been developed, which are based on polynomial and spline collocation. They outperform even integral equation methods for classical diffraction with respect to accuracy and computing time. These results paved the way for a cooperation with the company International Intellectual Group, Inc., USA, on consultation and software development for conical diffraction problems.

An important event in 2008 was the organization of the workshop "Phase Transitions and Optimal Control", together with the Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*. In a lively atmosphere, 70 participants from 15 countries discussed new developments in this exciting field at the interface of materials science, analysis, optimization, and numerics.

In the sequel, further scientific achievements of the research group in 2008 are detailed.

Optimization and optimal control

The ongoing research in the areas of stochastic and nonsmooth optimization was mainly motivated by the MATHEON project C7 "Mean-risk models for electricity portfolio management and stochastic programming", but also related to a Ph.D. thesis supervised in GRK 1128. A major progress was achieved in scenario reduction for mixed-integer stochastic optimization problems [6]. In particular, an algorithmic approach to scenario selection based on minimizing polyhedral discrepancies was formulated and implemented. In the context of nonsmooth optimization, recent work ad-

dressed the topics of uniform boundedness of convex processes as well as of normal cone and co-derivative calculus in the sense of Mordukhovich [7]. The latter is an important tool for characterizing stationary points in deterministic or stochastic equilibrium problems under equilibrium constraints (EPECs) as they arise from spot market models in electricity production. This topic has been intensively analyzed in the context of the MATHEON project C7. In particular, recently concluded work identifies stationarity conditions for EPEC solutions in markets regulated by an independent system operator (ISO).

Concerning the optimal control of PDEs, the work on a priori error estimates for finite element discretization of state-constrained problems has been continued. An account of the results achieved in the last years can be found in the Scientific Highlights article "Optimal control of partial differential equations with pointwise state constraints" by Christian Meyer on page 31.

A new topic of the research group in the field of optimal control is the optimization of elastoplasticity systems. In [5], the optimal control of static infinitesimal plasticity with linear kinematic hardening is discussed. Owing to the underlying plasticity model, one is faced with an optimal control problem governed by a variational inequality. Such optimal control problems are known to provide particular difficulties due to their nonsmooth character. A common approach is the Yosida approximation of the maximal monotone map associated with the variational inequality and, in case of elastoplasticity, this amounts to the well-known viscoplastic approximation. The preprint investigates this approximation and shows convergence of the approximate optimal solutions to the optimal solution of the original problem.

In cooperation with Antonio Fasano (University of Florence), a mathematical model for the case hardening of steel has been proposed and analyzed. Carbon is dissolved in the surface layer of a low-carbon steel part at a temperature sufficient to render the steel austenitic, followed by quenching to form a martensitic microstructure. The model consists of a semilinear evolution equation for the temperature and a quasilinear evolution equation for the carbon concentration, both coupled with two ordinary differential equations to describe the evolution of phase fractions. In [4], questions of existence and uniqueness of solutions are investigated. The model gives rise to a number of interesting control problems, which will be investigated in the future.

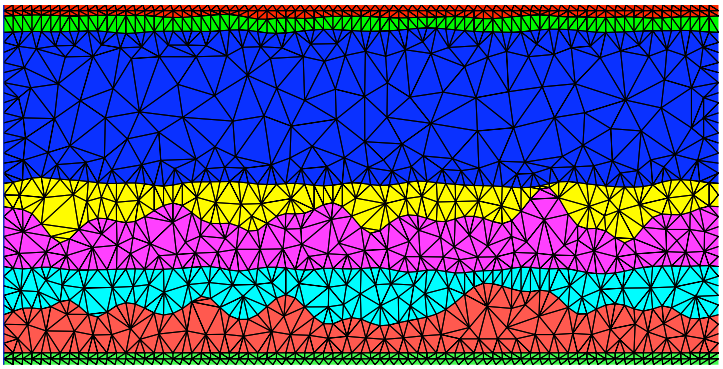


Fig. 1: *Simulated multilayer system*

Inverse problems

The cooperation with the Physikalisch-Technische Bundesanstalt (PTB) on inverse problems for the scatterometric measurement of photolithographic masks was continued in the framework of the project "CDuR 32" funded by the Federal Ministry of Education and Research. The main contribution will be to develop a reconstruction algorithm for the geometrical parameters (heights, critical dimensions, side-wall angles) of three-dimensional biperiodic structures. Clearly, the first step is the simulation of the scattered electromagnetic fields. In 2008, the finite element method (FEM) code "ngsolve" has been adapted to the solution of the time-harmonic Maxwell system over grating structures. Another problem is the gap still existing between experimental data and numerically computed parameters, which is due to model errors. In particular, the assumption of smooth interfaces seems to be violated. To check the reliability of the multilayer system model, a Monte Carlo approach to layer systems with rough interfaces has been implemented. Figure 1 depicts a randomly generated multilayer system. With this code, it can be shown that the multilayer simulations by the standard IMD software based on modified Fresnel formulae are acceptable for a multilayer system of pairs of molybdenum/silicon layers. In the case of refined systems of quadruplets with intermediate layers simulating diffusion zones, remarkable differences between IMD and FEM/Monte Carlo methods can be found (cf. Figure 2).

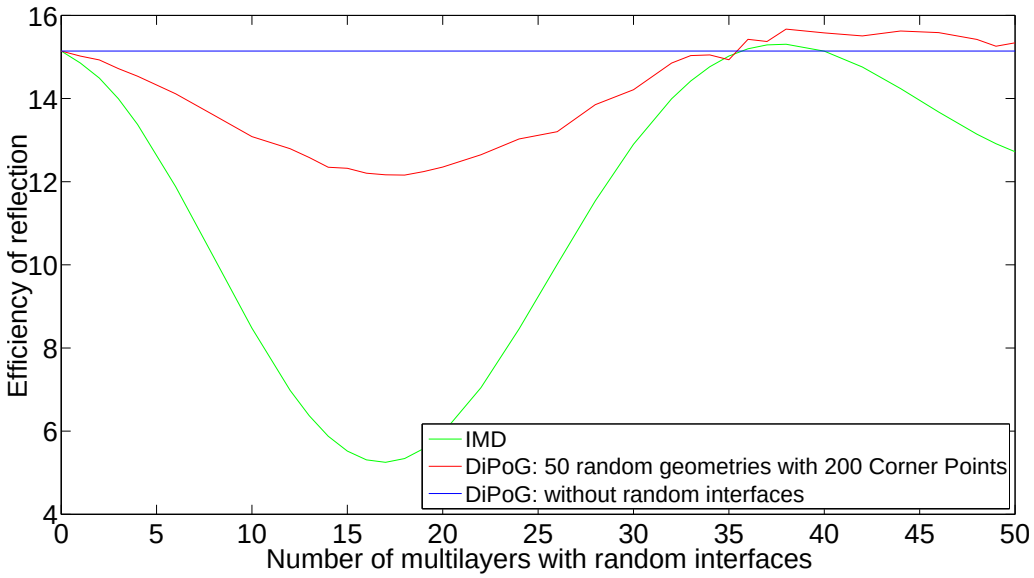


Fig. 2: *Reflectivity of multilayer simulations*

In cooperation with Simon N. Chandler-Wilde (University of Reading), a new variational approach in weighted Sobolev spaces for the analysis of rough-surface scattering problems has been studied. Problems of this type arise frequently in applications, for example, in diffractive optics and in modeling acoustic and electromagnetic wave propagation over outdoor ground and sea surfaces. The problem studied is the scattering of time-harmonic acoustic waves by an unbounded sound-soft rough surface, where the scattering surface is assumed to lie within a finite distance of a flat plane. The variational formulation of this problem is set in a layer of finite thickness between the surface and some flat plane lying above that surface on which the solution is required to satisfy

a nonlocal boundary condition involving the exact Dirichlet-to-Neumann map. As the main result, it could be shown that the problem is well posed in an energy space with weights decaying or increasing polynomially as a function of radial distance within the layer [1]. In particular, this covers existence and uniqueness of solutions in the practically important cases of incident plane waves in two and incident cylindrical waves in three space dimensions.

The cooperation with George Hsiao (University of Delaware) on the interaction between an elastic body and a compressible inviscid fluid occupying the unbounded exterior domain also continued. The inverse problem of determining the shape of such an elastic scatterer from the measured far-field pattern of the scattered fluid pressure field is of central importance in detecting and identifying submerged objects. In 2008, a new reconstruction method has been developed, approximating the acoustic and elastodynamic waves by simple layer potentials and reformulating the inverse problem as an optimization problem. It was proved that the optimization problem has a solution and that, for the regularization parameter tending to zero, the minimizers tend to a solution of the inverse problem [3]. In contrast to a previous finite element-based approach [2], the presented method does require neither a direct solution method nor an additional treatment of possible Jones modes.

References

[1] S.N. Chandler-Wilde, J. Elschner, *Variational approach in weighted Sobolev spaces to scattering by unbounded surfaces*, in preparation.

[2] J. Elschner, G.C. Hsiao, A. Rathsfeld, *An inverse problem for fluid-solid interaction*, Inverse Probl. Imaging, **2** (2008), pp. 83–120.

[3] J. Elschner, G.C. Hsiao, A. Rathsfeld, *An optimisation method in inverse acoustic scattering by an elastic obstacle*, WIAS Preprint no. 1365, 2008, submitted.

[4] A. Fasano, D. Hömberg, L. Panizzi, *A mathematical model for case hardening of steel*, to appear in: Math. Models Methods Appl. Sci.

[5] R. Griesse, C. Meyer, *Optimal control of static plasticity with linear kinematic hardening*, WIAS Preprint no. 1370, 2008.

[6] R. Henrion, C. Küchler, W. Römisch, *Discrepancy distances and scenario reduction in two-stage stochastic integer programming*, J. Indust. Management Optim., **4** (2008) pp. 363–384.

[7] R. Henrion, J. Outrata, *On calculating the normal cone to a finite union of convex polyhedra*, Optimization, **57** (2008), pp. 57–78.

[8] G. Schmidt, *Integral equations for conical diffraction by coated gratings*, to appear in: J. Integral Equations Appl.

3.5 Research Group 5 *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.

In 2008, there were significant activities in the field of graduate education. The DFG International Research Training Group "Stochastic Models of Complex Processes and their Applications", coordinated by Anton Bovier, has operated successfully. Two Ph.D. theses were completed: by Andrej Depperschmidt on "Survival, complete convergence and decay of correlations for a spatial branching system with local regulation" and by Anton Klimovski on "Sums of correlated exponentials: Two types of Gaussian correlation structures" (both supervised by Anton Bovier). Two Weierstrass postdoctoral fellows, Giada Basile and Olivier Zindy, successfully worked in the group.

In 2008, the research group was involved in the organization of several international conferences. Anton Bovier acted as organizer and chair of the invited session "Stochastic Processes in Physics" at the *7th World Congress in Probability and Statistics* in Singapore. He also co-organized workshops on "Metastability" in Eindhoven and on "Random Systems from Physics to Biology" in Berlin. A particular highlight of the year was the Mini-workshop "Numerics for Kinetic Equations" at the Mathematical Research Institute in Oberwolfach, organized by Wolfgang Wagner together with Irene Gamba (Austin) and Sergej Rjasanow (Saarbrücken).

Fig. 1: *Participants of the Mini-workshop "Numerics for Kinetic Equations" at the Mathematical Research Institute in Oberwolfach*

The year 2008 was marked by significant changes in the group's composition. In January, Anton Bovier received a call to a full professorship at the University of Bonn, where he finally moved in October. This is a severe loss for our institute, where he had been working since 1992. Two more

permanent members of the group left WIAS: Patrik Ferrari moved to Bonn, and Louis-Pierre Arguin got a position at the Courant Institute, New York University.

To conclude the overview of last year's event, some scientific achievements will be outlined below. Significant progress has been achieved in the field of stochastic models for population genetics. Concerning these results, the reader is referred to the article by Matthias Birkner in the Scientific Highlights section of this report on page 38.

Stochastic dynamics for spin systems

The mathematical analysis of random systems originating from Statistical Physics has been a key focus of the research group over the last decade. While classical theory concentrated on equilibrium properties of the systems, more recently, emphasis has shifted toward dynamical questions. A particularly important phenomenon is *metastability* related to the transition from a local equilibrium to a global one. The so-called *potential theoretic approach* to metastability that was developed in [5], [6] has led to a unified treatment of metastability in many different models and has allowed to improve the precision of estimates of key quantities. Significant progress has been achieved in this project during the last year.

Precise estimates for the transition time between the metastable state and the stable state were obtained in [3]. Both Ising spin systems subject to Glauber spin-flip dynamics and lattice-gas particle systems subject to Kawasaki hopping dynamics were studied. In [2], the metastability phenomenon in random spin systems was investigated. A new method to obtain matching upper and lower bounds on metastable times was developed, based on the potential theory approach. Applying this technique to the random field Curie–Weiss model, sharp asymptotics on the metastable times at any temperature were obtained.

In the last decade, the remarkable connection between mixing time (the number of steps until the dynamics is close to its equilibrium measure) and equilibrium phase transitions has been a central object of research. One of the main questions left open by the dynamical analysis is the influence of boundary conditions on the mixing time and its dependence on the underlying graph structure (see Figure 2). A sharp dependence of the mixing time on the boundary conditions for the Ising model on nonamenable graphs was proved in [1].

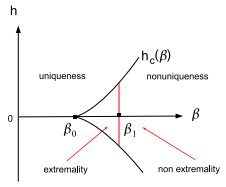


Fig. 2: *Phase transition diagram for the Ising model on a tree graph*

Microscopic modeling of stock markets

The goal of this project is to get a deeper understanding of the underlying market mechanisms that cause statistical properties of the price process, observable in different markets and on different time scales, also called *stylized facts*. An agent-based model on the level of order book dynamics has been introduced in [4], called *the opinion game*. Simulations in this model raised questions concerning the stability of markets subject to model parameters describing essentially the behavior of long-term investors.

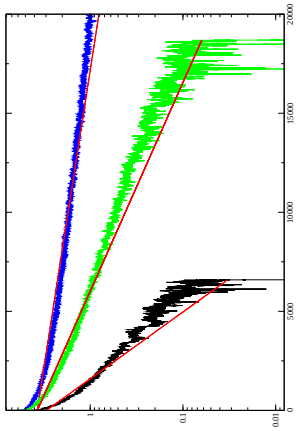


Fig. 3: *Finding the right parameters for the optimal execution problem: Simulations and regression lines (red)*

The analysis of the *opinion game* with a particular focus on the stability of the system with respect to certain parameters provided a simple but analytically treatable model for the behavior of long-term investors. A detailed analytical investigation of this simpler model with remarks and conclusions for the *opinion game* can be found in [8].

There is another way to look at microscopic market models. Since these models provide realistic responses to events in the market, they can be used as a qualitative benchmark for problems concerning the maximization of profit or the minimization of costs, respectively, under certain constraints. An example for a cost minimization problem is the question about the optimal execution of large orders. Here, a trader would like to purchase a huge volume of shares within a finite time horizon. As the volume of shares for the current market price is limited, the trader's order leads to an undesirable rise of the price. This extra impact on the price can be reduced by splitting the volume to purchase into smaller orders, which the trader executes at certain points in the given time interval. It is empirically known that the price relaxes after the execution of a large order, and thus, the extra impact decreases. Considerable progress has been achieved in the study of optimal strategies.

Stochastic particle methods for rarefied gas flows

The purpose of this project is to study the relationship between stochastic interacting particle systems and solutions of nonlinear kinetic equations. These equations are crucial for an adequate description of many processes of scientific and industrial importance. In recent years, there have been intensified research activities in the field of numerical algorithms for kinetic equations related to new areas of application. Typical gas flows in micro- and nanomachines are in the rarefied regime, and therefore the classical Boltzmann equation is often used to model such flows.

On the one hand, results on the asymptotic behavior of the particle system (when the number of particles increases) provide insight into properties of the solution. On the other hand, appropriate stochastic particle systems are used for the numerical treatment of the macroscopic equation. Stochastic numerical methods provide results that are subject to random fluctuations. There are significant numerical challenges related to the novel applications mentioned above. In low Mach number rarefied flows, there is a very small signal-to-noise ratio. Thus, the construction of algorithms with reduced fluctuations is an important issue (variance reduction problem).

The paper [7] describes the deviational particle Monte Carlo method for the Boltzmann equation. The approach is an application of the general "control variates" variance reduction technique to the problem of solving a nonlinear equation. The deviation of the solution from a reference Maxwellian is approximated by a system of positive and negative particles. Previous results from the literature are modified and extended. New algorithms are proposed that cover the nonlinear Boltzmann equation (instead of a linearized version) with a general interaction model (instead of hard spheres). The limiting equations reflect the influence of various numerical approximation parameters. Detailed simulation schemes are provided for the variable hard-sphere interaction model. This approach was one of the "hot topics" discussed during a recent mini-workshop in Oberwolfach (cf. Figure 1).

References

[1] A. Bianchi, *Glauber dynamics on hyperbolic graphs: Boundary conditions and mixing time*, Electron. J. Probab., **13** (2008), pp. 1980–2012.

[2] A. Bianchi, A. Bovier, D. Ioffe, *Sharp asymptotics for metastability in the random field Curie–Weiss model*, WIAS Preprint no. 1342, 2008, submitted.

[3] A. Bovier, F. den Hollander, C. Spitoni, *Homogeneous nucleation for Glauber and Kawasaki dynamics in large volumes at low temperatures*, WIAS Preprint no. 1331, 2008.

[4] A. Bovier, J. Černý, O. Hryniv, *The opinion game: Stock price evolution from microscopic market modelling*, Int. J. Theor. Appl. Finance, **9** (2006), pp. 91–112.

[5] A. Bovier, M. Eckhoff, V. Gayrard, M. Klein, *Metastability in stochastic dynamics of disordered mean-field models*, Probab. Theory Related Fields, **119** (2001), pp. 99–161.

[6] ———, *Metastability and low lying spectra in reversible Markov chains*, Comm. Math. Phys., **228** (2002), pp. 219–255

[7] W. Wagner, *Deviational particle Monte Carlo for the Boltzmann equation*, Monte Carlo Methods Appl., **14** (2008), pp. 191–268.

[8] A. Weiss, *Escaping the Brownian stalkers*, WIAS Preprint no. 1304, 2008, to appear in: Electron. J. Probab.

3.6 Research Group 6 *Stochastic Algorithms and Nonparametric Statistics*

The research of the group is organized in the research projects Statistical Data Analysis and Applied Mathematical Finance. 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 valuation in financial markets using efficient stochastic algorithms.

The research group has reached a leading position with important mathematical contributions and the development of statistical software. Part of the research is carried out within the three MATHEON projects A3, A10, and E5, and the SFB 649 projects B5 and B7 (see page 96). Members of the group were involved in several industrial contracts. New pricing methods for Bermudan products have led to a continued collaboration with the Landesbank AG. The problem of pricing and calibration of different financial instruments is the subject of a collaboration with two other banks: Nordbank and Westdeutsche Genossenschafts-Zentralbank. The group also participates in a contract with ALSTOM (Switzerland) Ltd., on "Gas turbine process simulation". The contribution concentrates on general statistical modeling and Monte Carlo approximations.

Scientific highlights achieved by the research group in 2008 are provided below.

Statistical data analysis

The focus within the project area Statistical Data Analysis is on methods that automatically adapt to unknown structures using some weak qualitative assumption. This includes structural adaptive smoothing and methods for dimension reduction. The current research focuses on nonasymptotic exponential risk bounds with applications to parameter tuning for the nonparametric estimation, models selection and testing; see [6].

The main fields of application are econometrics, mainly pursued within subprojects of the DFG Collaborative Research Center SFB 649, and medical imaging. Within subproject A3 "Image and signal processing in medicine and biosciences" of the DFG Research Center MATHEON, the group focuses on applications in neuroscience.

Structural adaptive methods for general smoothing and imaging problems have been implemented as packages `AWS` and `adimpro` within the R-Project for Statistical Computing.

Functional magnetic resonance imaging (fMRI). Functional magnetic resonance imaging (fMRI) is the most informative tool for the in vivo examination of human brain function on small spatial scales. It is utilized both in research as well as in clinical applications, such as diagnosis and treatment of brain lesions. The analysis of fMRI data requires a substantial use of statistical models and methods.

Smoothing is used in this context for signal enhancement and to provide a solution to the multiple test problem in signal detection. The collaboration with partners, e.g., from Cornell University, has been continued on the analysis of functional magnetic resonance experiments, leading to new applications, extensions, and refinements of our methods, and to new interesting problems. The advantages of the group's smoothing methodology on patient data could be proved; see Figure 1 and, e.g., [5]. Special emphasis has been on problems in high-resolution fMRI. Requirements from applications have led to a further refinement of the R-package `fmri`.

The collaboration with the eVITA Project "Scale-space Methods and GMRFs with Applications", University of Tromsø, on medical imaging problems includes computer-aided diagnostics and telemedicine applications.

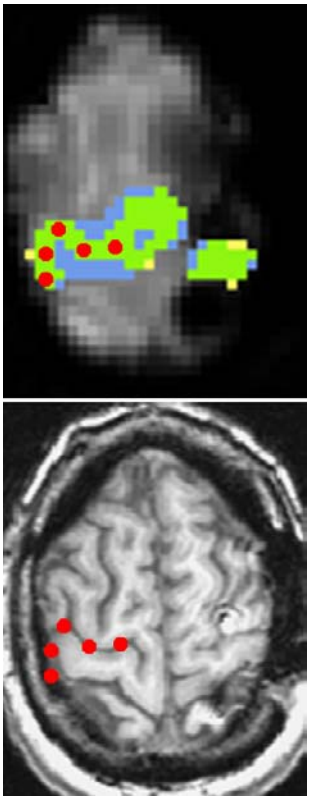


Fig. 1: *Spatially accurate detection (green and yellow) in contrast to nonadaptive smoothing (green and blue)*

Diffusion weighted magnetic resonance imaging (DWI/DTI). Diffusion weighted imaging (DWI) has become an important tool to investigate fiber structure in tissue. In neuroscience, it is used to measure anisotropy of water diffusion, which is believed to correspond to the anatomical structure in the white matter area of the brain. The spatial distribution of strength and main directions of anisotropy is used, e.g., for diagnosis of stroke and surgical planning. Further research interests include fiber tracking and investigation of brain connectivity.

The common description of anisotropy is based on the diffusion tensor (DTI) model. Data obtained in DWI are characterized by a high noise level. Thus, the estimation of quantities like anisotropy indices or the main diffusion direction may be significantly compromised by noise. In [4], the group's methods for analyzing DWI data within the DTI framework were extended by using a heteroskedastic nonlinear tensor model, appropriate variance modeling, and corrections for the Rician bias, leading to significantly improved results. Figure 2 on the next page provides a comparison of voxelwise and adaptively smoothed tensor estimates using an artificial example. The R-package `dti` now contains functions to perform the whole DTI analysis including two- and three-dimensional visualization of results.

Applied mathematical finance

The project focuses on the solution of challenging mathematical problems motivated by applications in the *financial industry*. The development and rigorous mathematical analysis of innovative methods and algorithms based on fundamental stochastic principles are of primary interest.

Many areas in financial modeling utilize optimal control theory, and there is an increasing demand for solutions to optimal control problems for real-world financial problems, which are both accurate and effective. In [2], several regression algorithms for solving general stochastic optimal control problems via Monte Carlo were developed. This type of algorithms is particularly useful for problems with a high-dimensional state space and a complex dependence structure of the underlying Markov process with respect to some control. The main idea behind the algorithms is to simulate a set of trajectories under some reference measure and to use the Bellman principle combined with fast methods for approximating conditional expectations and functional optimization.

Theoretical properties of the presented algorithms are investigated, and the convergence to the optimal solution is proved under mild assumptions.

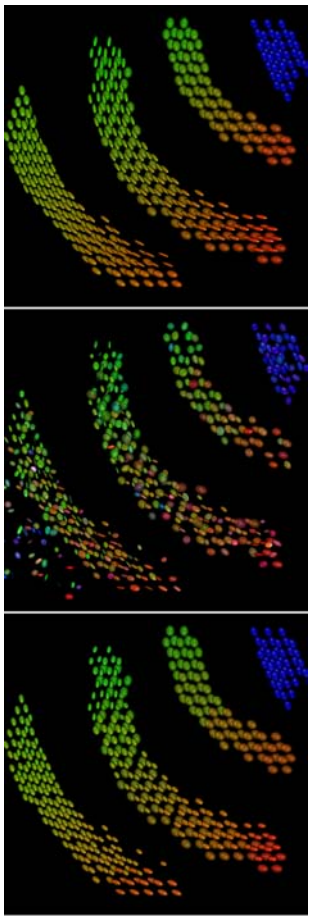


Fig. 2: *Artificial DTI example. Top: true tensors, center: voxelwise estimates, bottom: adaptive smoothing*

Financial modeling with affine processes became very popular in the recent literature due to their rich dynamics and implied volatility patterns. Generally, the characteristic function of an affine jump diffusion may be represented as the solution of a nonlinear Ricatti differential equation. However, such an equation can be solved analytically only in a few special cases and numerically only in low dimensions. Therefore, new approximation methods for computing the characteristic function in an efficient way are called for. In [1], a new approach by considering classes of holomorphic transforms of the state space vector, which are holomorphic in some neighborhood of time zero and the positive real line, is proposed. Via such transforms, functional series expansions are derived that allow for effective computation of the characteristic function. In particular, in the context of option pricing, these expansions apply to general affine price processes in the presence of jumps.

References

[1] D. Belomestny, J. Kampen, J. Schoenmakers, *Holomorphic transforms with application to affine processes*, WIAS Preprint no. 1297, 2008, submitted.

[2] D. Belomestny, A. Kolodko , J. Schoenmakers, *Regression methods for stochastic control problems and their convergence analysis*, WIAS Preprint no. 1392, 2009, submitted.

[3] J. Kampen, A. Kolodko, J. Schoenmakers, *Monte Carlo Greeks for financial products via approximative transition densities*, SIAM J. Sci. Comput., **31(1)** (2008), pp. 1–22.

[4] J. Polzehl, K. Tabelow, *Structural adaptive smoothing in diffusion tensor imaging: The R package dti*, WIAS Preprint no. 1382, 2008, submitted.

[5] K. Tabelow, J. Polzehl, A.M. Ulug, J.P. Dyke, R. Watts, L.A. Heier, H.U. Voss, *Accurate localization of brain activity in presurgical fMRI by structure adaptive smoothing*, IEEE Trans. Med. Imaging, **28** (2008), pp. 531–537.

[6] V. Spokoiny, *Multiscale local change point detection with applications to Value-at-Risk*, Ann. Statist., in print.

3.7 Research Group 7 *Thermodynamic Modeling and Analysis of Phase Transitions*

Overview

The essential topics of the research group may be found within the three categories

- Production and application of modern materials
- Energy technology
- Multi-scale problems and, in particular, thin films

From a mathematical point of view, the research group studies initial boundary value problems for coupled nonlinear partial differential equation (PDE) and ordinary differential equation (ODE) systems with special focus on free boundary problems. The physical background of those systems are phase transitions, hysteresis, evolution of thin films, transport of matter, diffusion problems in liquids as well as in crystals, and nucleation of droplets and bubbles.

The complexity of the treated problems arise due to various strong couplings, for example, interface motion producing mechanical stresses, changing electromagnetic fields influencing flow patterns, chemical reactions and the appearance of precipitates in crystals leading to lattice deformations, nonlocal radiation fields interacting with non-convective heat conduction, and long-range interatomic interactions leading to nonlocal PDEs.

Highlights

1. The interdisciplinary project KRIST$\widetilde{MAG}$® has been completed with great success in July 2008. Two industrial companies, physicists, engineers, and mathematicians have designed new heater-magnet modules to control the melt flow and the shape of the melt-crystal interface during crystal growth. Three devices for crystal growth are now available, there are five patents, and the WIAS group has initialized the application for a sixth patent. The project was honored in December 2008 with the “Innovation Prize Berlin-Brandenburg 2008”.

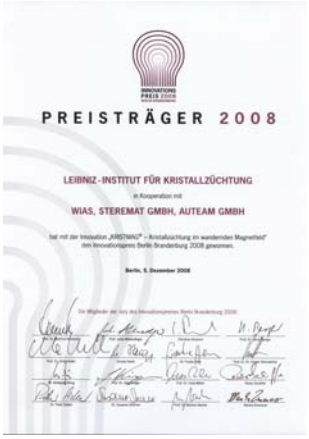


Fig. 1: *Innovation Prize Berlin-Brandenburg 2008*

Five members of the research group contributed to the project. Jürgen Sprekels and the principal investigators Olaf Klein and Christiane Lechner did most of the work concerning the numerical simulations of the growth device. Based on OpenMP, Christiane Lechner improved the three-dimensional version of the software NAVIER for its use on *shared-memory machines*, and she developed a tool to perform *large eddy simulations* that are based on the *Smagorinski viscosity model*.

Wolfgang Dreyer accounted for some modeling of the PDE system at hand consisting of the coupled system of Navier–Stokes equations, the heat equation including radiation, and reduced Maxwell equations. Its analysis was carried out by Pierre-Étienne Druet within the framework of a Ph.D. thesis [2], and Peter Philip improved the software code `WIAS-HiTNIHS`, which calculates the

transport of heat in devices with cylindrical symmetry with a special focus on heat radiation and temperature-dependent material properties.

2. The study on *Online Control of Piezo-electrical Actuators* has likewise been finished in 2008. The German Patent and Trade Mark Office gave a patent to Pavel Krejčí, Klaus Kuhnen (Robert Bosch GmbH), and Heinz Janocha (University of Saarland) for a method for online control of nonlinearities that influence the transfer behavior of actuators. The new method allows real-time compensation in the low frequency range of unwanted oscillations, which are accompanied by hysteretic phenomena. From a mathematical point of view, the problem is related to the exact control of a beam equation with a hysteretic constitutive law.

3. Pavel Krejčí and Dietmar Hömberg (Research Group *Nonlinear Optimization and Inverse Problems*), jointly with Martin Brokate (Munich), Pierluigi Colli (Pavia), and Dan Tiba (Bucharest), organized the International Workshop "Phase Transitions and Optimal Control" at WIAS from October 23–25, 2008 (see page 102). The workshop was related to the main research lines of Jürgen Sprekels, who celebrated his 60th birthday that week.

4. Within the group's newly developed framework *Mathematics in Industry*, Barbara Wagner jointly with Andreas Münch (University of Nottingham), Bernd Rech (Hahn–Meitner Institute, Berlin) and Volker Mehrmann (Technical University of Berlin and DFG Research Center MATHEON) organized from October 6–9 the Workshop "Technologies of Thin Film Solar Cells"; see page 102.

On its first day, four industrial companies presented various problems in the context of highly efficient thin-film solar cells that were then studied in detail, and after four days, first solutions were presented. The workshop has lead to various longer-term collaborations between applied mathematics and industry.

5. Christiane Kraus and Dorothee Knees (Research Group *Partial Differential Equations*) successfully applied for a three-year funding within the competitive procedure of the Leibniz Association. In 2009–2011, they will run the new Leibniz Group "Modeling of Damage Processes" at WIAS that is devoted to the modeling and analysis of failure processes in materials. In particular, it is intended to compare the classical theories of failure with a new approach that describes, for example, the evolution of cracks by phase field models. Details may be found in the Scientific Highlights article "A Gibbs–Thomson Law with Anisotropic Surface Tension and Elasticity" by Christiane Kraus on page 26.

Funded projects with industry collaboration

1. The KRIST*MAG*® project has generated several new ideas that can likewise be used to develop new crystal growth systems for the production of solar silicon. Here, the speciality is the increasing demand for large block-shaped crystals. To this end, the consortium AVANT*SOLAR* (**A**nlagen- und **V**erfahrensentwicklung sowie **A**bsatz einer **n**euen **T**echnologie zur Kristallisation von ***Solar***-Silizium, equipment and process development as well as sale of a new technology for the crystallization of solar silicon) was founded, including a large German industrial producer of photovoltaic cells. The project runs for three years, and the research group contributes with two full positions with industrial funding. The new challenges for the WIAS team, headed by Wolfgang Dreyer, Olaf

Klein, and Jürgen Sprekels, are simulations based on the coupled three-dimensional system of Navier–Stokes equations, diffusion equations with chemical reactions, Maxwell's equations, and the heat conduction equation. Special emphasis must be placed on controlling a homogenous distribution of unwanted impurities in melt and crystal and guaranteeing an appropriate geometric shape of the crystal-melt interface. In particular, a control of the triple point, where the interface meets the wall of the crucible, is of fundamental importance. The project benefits from the support provided by the Research Group *Numerical Mathematics and Scientific Computing* and Eberhard Bänsch (University of Erlangen). Moreover, Pierre-Étienne Druet from the MATHEON subproject C9 "Numerical simulation and control of sublimation growth of semiconductor bulk single crystals" and Margarita Naldzhieva from C14 "Macroscopic models for precipitation in crystalline solids" make important contributions to the analysis of the optimization of conduction heating (C9) and to the "triple point" problem (C14).

2. Barbara Wagner and Ernst Höschele, in collaboration with Andreas Münch (University of Nottingham), have continued an industry-funded project, financed until April 2010, which concerns the dynamical contact problem between an elastomer substrate and a liquid film. Due to the deformation of the substrate, one is here confronted with a free boundary problem of extreme numerical complexity. In 2008, Ernst Höschele developed the software NHS for finite element discretization of a neo-Hookean material with incompressibility. Furthermore, the simulation of the liquid is based on the software NAVIER, and a combination of both codes solves the problem completely. After an intricate validation of the results, the industrial partner was trained to use the new combined software product.

3. Jointly with an industrial producer of semi-insulating GaAs wafers, the modeling, simulation, and analysis of the dissolution of unwanted precipitates appearing during heat treatment in gallium arsenide (GaAs) wafers has been continued [5]. This topic is also funded with two positions within the MATHEON subproject C14 "Macroscopic models for precipitation in crystalline solids", which is headed by Wolfgang Dreyer and Barbara Niethammer (University of Oxford). In 2008, the following three different topics were considered: 1. The dissolution of precipitates according to three different models has been compared: (i) Dissolution of a single precipitate due to diffusion in its surroundings, (ii) Dissolution of an ensemble of many precipitates according to the Becker–Döring ODE system, and (iii) according to a homogenized version of a coupled PDE system of parabolic diffusion equations and the elliptic quasi-static momentum balance with a more involved boundary condition at the free interface between precipitate and crystal. 2. The Becker–Döring system predicts a metastable state in the supersaturated regime, where the production rates of precipitates are almost constant and equal to each other. The crucial quantity is the time lag to reach the metastable state from given initial data. In 2008, it was found that the accepted strategy to calculate the time lag contained a serious error that was analyzed and could be corrected by Wolfgang Dreyer, Margarita Naldzhieva, and Frank Duderstadt. 3. Furthermore, that team, in collaboration with Stefan Eichler (Freiberger Compound Materials GmbH), modeled the conduction of heat in the vicinity of the triple line of a *vertical gradient freeze* device, where the crystal-melt interface meets the crucible wall. The mathematical problem is stationary heat conduction within a convex domain with corners that contains a free boundary described by a Gibbs–Thomson law [7].

Funded under Priority Programs of the German Research Foundation

1. Within the Priority Program SPP 1164 "Nano- & Microfluidics: Bridging the Gap between Molecular Motion and Continuum Flow", Barbara Wagner, Konstantin Afanasiev, and Dirk Peschka, in collaboration with Andreas Münch and John King (both School of Mathematical Sciences, University of Nottingham), continued work on the problem of "Mathematical modeling, analysis numerical simulation of thin films and droplets on rigid and viscoelastic substrates, emphasizing the role of slippage". A hierarchy of PDE and ODE models to simulate the evolution of droplets at rigid substrates was developed and tested by a new remeshing algorithm that allows one to simulate flow problems in strongly deformable domains with free boundaries. The algorithm is now implemented in the code NAVIER. In addition to this topic, a new hierarchy of models is studied with the intention to manipulate non-Newtonian liquid films by an electrostatic field. For its completion, a proposal within the Individual Grants Program of the German Research Foundation is in preparation.

2. Funded by the Priority Program SPP 1095 "Analysis, Modelling and Simulation of Multiscale Problems", Wolfgang Dreyer and Antonio Segatti concluded research on the transition of discrete lattice models described by a large ODE system to a few effective PDEs. In the thermodynamics, according to Whitham's system, irreversibility exclusively was found when shocks appeared. In order to study the origin of irreversibility for smooth solutions, a harmonic chain with an impurity was considered, more precisely, a harmonic chain in which the masses of the particles are normalized to 1, except for one heavy particle, which has mass M. For M large and a corresponding hyperbolic scaling of time, space, and particle index, a rigorous investigation of the macroscopic behavior of such an arrangement has lead to an ODE-PDE system consisting of a PDE for the light particles that is coupled to an ODE for the heavy particle, which exhibits exponential decay and thus describes irreversible behavior. The results are given in detail in [6].

Selected research topics in detail

1. In addition to the patent on *Online Control of Piezo-electrical Actuators*, the research on hysteresis phenomena was highlighted by the paper [3] by Ronald B. Guenther (Oregon State University), Pavel Krejčí, and Jürgen Sprekels, who were able to generalize results for elastic-plastic beams, obtained in 2007, to small strain oscillations of elastic-plastic Kirchhoff plates. Based on a three-dimensional von Mises flow rule, the corresponding Prandtl–Ishlinski operator could be completely characterized, and its weight function has been determined. The existence of solutions and uniqueness results of the ensuing dynamical problem could be proved. As usual in the two-dimensional plate reduction of a three-dimensional body, the original five-dimensional space of stress deviators is reduced to three dimensions. However, obviously the original single yield condition appears now under an integral over the layers of the plate, so that the elastic-plastic transition does not happen simultaneously in each layer. As already shown by many other applications, the advantage of the Prandtl–Ishlinski setting lies in the possibility of a viscous regularization of the Prandtl–Ishlinski operator implying a simple and robust numerical method to solve the elastic-plastic problem, which is superior to the classical engineering approach.

2. The study on sharp interface limits of phase field models in various applications has been con-

tinued and intensified by Wolfgang Dreyer, Christiane Kraus, Robert Huth, Clemens Guhlke, Antonio Segatti, and a Ph.D. student, Thomas Petzold, from the Research Training Group (GRK) 1128 "Analysis, Numerics, and Optimization of Multiphase Problems" at the Humboldt University of Berlin. Among the applications are (i) the storage of hydrogen in hydrides, (ii) simulations for an improved design of the cathode of lithium-ion batteries, (iii) $\gamma - \alpha$ transitions and the formation of unwanted cementite in steel, (iv) the design and production of new lead-free solder joints in microelectronic devices, (v) the formation and evolution of unwanted vapor bubbles in flowing water [8].

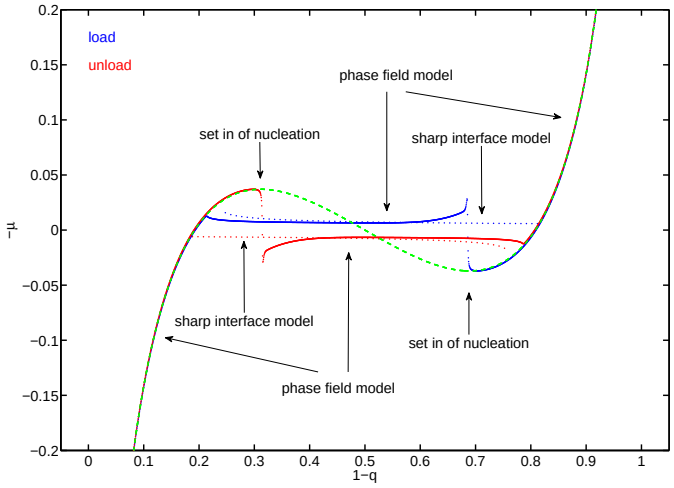


Fig. 2: *Sharp interface model of a lithium-ion cathode in juxtaposition to a possible phase field model. Vertical axes: chemical potential, horizontal axes: mass of charge*

These applications have the appearance of phase transitions in common that might be accompanied by hysteresis. It has become evident that the following strategy for an appropriate modeling is mandatory here: 1. Determine the possible equilibria of the phenomena. 2. If hysteresis appears, determine whether it runs through equilibrium states. 3. Describe the evolution to equilibrium by a sharp interface model. 4. Regularize this model by guessing higher derivatives so that a phase field model results. 5. Perform its sharp interface limit and check whether there results the correct sharp interface model from step 3.

3. In the subproject C10 "Modeling, asymptotic analysis and numerical simulation of the dynamics of thin film nanostructures on crystal surfaces" of the DFG Research Center MATHEON, Maciej Korzec, Pete Evans, and Barbara Wagner, jointly with Andreas Münch (University of Nottingham), continued modeling the epitaxic growth of quantum dots by an extended Cahn–Hilliard equation of sixth spatial order for the profile of the structure; see [4]. In 2008, this equation has been further generalized to take into account anisotropy and mechanical interactions of pyramidal quantum dots. In particular, the appearance of the variational derivative of the surface free energy introduces a tremendous complexity into the coupled system of the elasticity equation for the mechanical displacement and the generalized sixth-order Cahn–Hilliard equation for the height of the pyramids. Parallel to the modeling, a new numerical method has been established that relies on pseudospectral theory.

Ph.D. students

Wolfgang Dreyer, Jürgen Sprekels, and Barbara Wagner, jointly with other partners, guide and supervise 15 Ph.D. students. Their studies are carried out within the DFG Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", within the DFG Research Center MATHEON "Mathematics for key technologies", and in collaboration with the Technical University (TU) and the Humboldt University (HU) of Berlin.

In the year 2008, two Ph.D. students successfully defended their dissertations:

- Analysis of thin-film rupture including the effect of slippage (GRK 1128, supervisors: Münch (Nottingham)/Niethammer (Oxford)): Dirk Peschka passed his Ph.D. examination at HU Berlin with *magna cum laude*. The formation of interfacial singularities of fluid surfaces was studied by a two-dimensional reduction of a three-dimensional model that takes surface tension, intermolecular forces, and the Navier-slip boundary condition into account.

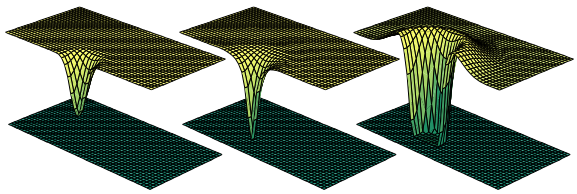


Fig. 3: *Two-dimensional simulation of the surface of a dewetted liquid film. Due to a van der Waals interaction between the liquid and the underlying substrate, an initially small disturbance grows and finally leads to an evolving rupture*

  The main novelties are (i) the systematic study of the effect of slippage with respect to singularity formation and transient solutions, (ii) the development of a numerical scheme that allows one to track physical singularities over many orders of magnitude, (iii) a rigorous mathematical study of the singularity formation for thin films, e.g., it was proved that singularities appear after a finite time, their shape was characterized, and convergence to self-similar solutions was proved.

- Investigations of microstructural changes in lead-free solder alloys by means of phase field theories (TU Berlin, Dreyer/Müller (TU)). Thomas Böhme passed his Ph.D. examination at the TU Berlin with *distinction*. The subject of his thesis concerned the simulation of the manufacturing of new lead-free solder materials for microelectronic devices. The essential breakthroughs are (i) the rational derivation of a new mixture theory of the eutectic alloy AgCu, (ii) the calculation of higher gradient terms by means of an atomistic lattice model, (iii) the simulation of spinodal decomposition and subsequent coarsening, (iv) experiments studying these phenomena and a comparison with theoretical results.

The following list gives ongoing Ph.D. studies with their current objectives:

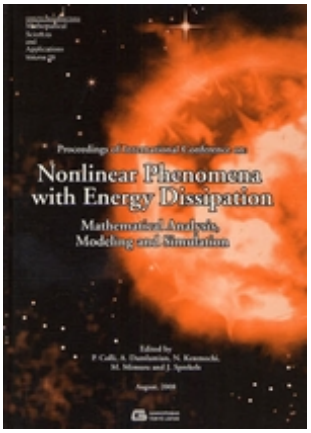
- Existence and uniqueness of a local phase field system with thermomechanical coupling (GRK 1128)
- Modeling, analysis and numerics of precipitation phenomena in steel (GRK 1128)
- Modeling, analysis and numerics of nucleation and evolution of bubbles in ternary mixtures in direct methanol fuel cells (GRK 1128)

- Coarsening of dewetted liquid droplets (GRK 1128): Details of this study may be found in the Scientific Highlights article “Dewetting of Complex Liquids” by Barbara Wagner on page 54.
- Numerics of Navier–Stokes equations (industry collaboration with funding)
- Evolution of quantum dots with extended Cahn–Hilliard equations (MATHEON C10)
- Modeling, asymptotic analysis and numerical simulation of the dynamics of thin film nanostructures on crystal surfaces (MATHEON C10)
- Existence, uniqueness and numerical simulations of the discrete Becker–Döring system and its continuous limit (MATHEON C14, industry collaboration with funding)
- Homogenization of a free boundary problem for the evolution of liquid precipitates in crystalline gallium arsenide (MATHEON C14)
- Existence and uniqueness of a magnetohydrodynamical system with heat conduction
- On the storage of hydrogen in hydrides (MATHEON C26)
- Mathematical modeling of lithium-ion batteries
- On cell proliferation

These topics rely on thermodynamic models of large complexity because they comprise various couplings of different phenomena. Examples are (i) diffusion and mechanical stresses, (ii) liquid flow in magnetic fields with heat conduction, (iii) complex thin film-substrate interactions. Thus, there arise involved initial-boundary value problems for nonlinear coupled systems of partial differential equations.

Miscellaneous

In 2008, Jürgen Sprekels, jointly with Karl Kunisch (Graz), Günter Leugering (Erlangen), and Fredy Tröltzsch (TU Berlin), organized the Workshop “Optimal Control of Partial Differential Equations” at the Mathematical Research Institute in Oberwolfach.



References

[1] P. COLLI, A. DAMLAMIAN, N. KENMOCHI, M. MIMURA, J. SPREKELS, EDS., *Proceedings of International Conference on: Nonlinear Phenomena with Energy Dissipation: Mathematical Analysis, Modeling and Simulation*, vol. **29** of Gakuto International Series Mathematical Sciences and Applications, Gakkōtosho, Tokyo, 2008, 475 pages.

[2] P.-E. DRUET, *Existence of weak solutions to the time-dependent MHD equations coupled to heat transfer with nonlocal radiation boundary conditions*, to appear in: Nonlinear Anal. Real World Appl.

[3] R.B. GUENTHER, P. KREJČÍ, J. SPREKELS, *Small strain oscillations of an elastoplastic Kirchhoff plate*, ZAMM Z. Angew. Math. Mech., **88** (2008), pp. 199–217.

[4] M.D. Korzec, P.L. Evans, A. Münch, B. Wagner, *Stationary solutions of driven fourth- and sixth-order Cahn–Hilliard type equations*, SIAM J. Appl. Math., **69** (2008), pp. 348–374.

[5] W. Dreyer, F. Duderstadt, *On the modelling of semi-insulating GaAs including surface tension and bulk stresses*, Proc. R. Soc. Lond., Ser. A, Math. Phys. Eng. Sci., **464** (2008), pp. 2693–2720.

[6] M. Herrmann, A. Segatti, *Infinite harmonic chain with heavy mass*, WIAS Preprint no. 1367, 2008, submitted.

[7] W. Dreyer, F. Duderstadt, S. Eichler, M. Naldzhieva, *On unwanted nucleation phenomena at the wall of a VGF chamber*, WIAS Preprint no. 1312, 2008, submitted.

[8] K. Hermsdörfer, Ch. Kraus, D. Kröner, *Interface conditions for limits of the Navier–Stokes–Korteweg model*, WIAS Preprint no. 1389, 2008, submitted.

A Facts and Figures

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

- Calls, Awards and Distinctions, Habilitations, Ph.D. Theses, Undergraduate-degree Supervision
- 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, Undergraduate-degree Supervision

A.1.1 Calls

1. A. Bovier, W3 professorship, January 21, Rheinische Friedrich-Wilhelms-Universität Bonn, Mathematisch-Naturwissenschaftliche Fakultät.
2. Ch. Meyer, Junior professorship, August 29, Rheinisch-Westfälische Technische Hochschule Aachen, Fakultät für Mathematik, Informatik und Naturwissenschaften.
3. ———, Junior professorship, October 1, Technische Universität Darmstadt, Fachbereich Mathematik and Graduate School of Computational Engineering.

A.1.2 Awards and Distinctions

1. O. Klein, *Innovation Prize Berlin-Brandenburg 2008*, December 5.
2. D. Knees, *Robert Bosch Stiftung: Fast Track Scholarship*, 2008–2010.
3. Ch. Lechner, *Innovation Prize Berlin-Brandenburg 2008*, December 5.
4. A. Mielke, *Coordinator of the Theoretical Mechanics Group of the Centro di Ricerca Matematica "Ennio De Giorgi", Pisa, Italy*.
5. ———, *Member of the Council of the International Society for Interaction of Mathematics and Mechanics (ISIMM)*.
6. J. Sprekels, *Chairman of the Board of Forschungsverbund Berlin e.V.*
7. ———, *Coordinator of the International Mathematical Science Institutes (IMSI)*.
8. ———, *Innovation Prize Berlin-Brandenburg 2008*, December 5.

A.1.3 Ph.D. Theses

1. Th. Böhme, *Investigations of microstructural changes in lead-free solder alloys by means of phase field theories*, Technische Universität Berlin, Institut für Mechanik, supervisor: Priv.-Doz. Dr. W. Dreyer, March 7.
2. A. Depperschmidt, *Survival, complete convergence and decay of correlations for a spatial branching system with local regulation*, Technische Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. A. Bovier, July 31.
3. A. Klimovski, *Sums of correlated exponentials: Two types of Gaussian correlation structures*, Technische Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. A. Bovier, June 24.
4. S. Heinz, *Preservation of quasiconvexity and quasimonotonicity in polynomial approximation of variational problems*, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. A. Griewank, July 18.
5. Th. Koprucki, *Zu kp-Schrödingeroperatoren*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. H. Gajewski, November 7.
6. D. Peschka, *Self-similar rupture of thin liquid films with slippage*, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. B. Niethammer, October 31.

7. F. Schmid, *Analysis of geometrically non-linear models for contact with dry friction*, Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. A. Mielke, July 2.
8. H. Si, *Three dimensional boundary conforming Delaunay mesh generation*, Technische Universität Berlin, Institut für Mathematik, supervisor: Prof. Dr. G.M. Ziegler, July 7.

A.1.4 Undergraduate-degree Supervision

1. J. Ankudinova, *Die numerische Lösung von nichtlinearen Black-Scholes-Gleichungen* (diploma thesis), Technische Universität Berlin, Institut für Mathematik, supervisor: Priv.-Doz. Dr. M. Ehrhardt, April 30.
2. B. Driehorst, *Berechnung der instationären, eindimensionalen Rohrströmung am Beispiel der Abgasrückführung* (diploma thesis), Technische Universität Berlin, Fachbereich Physikalische Ingenieurwissenschaften, supervisor: Priv.-Doz. Dr. M. Ehrhardt, April 22.
3. M. Liero, *Herleitung eines elastoplastischen Plattenmodells mit Methoden der Γ-Konvergenz* (diploma thesis), Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. A. Mielke, November 12.
4. M. Messerschmidt, *Wellen in inhomogenen Oszillatorketten* (bachelor thesis), Humboldt-Universität zu Berlin, Institut für Mathematik, supervisor: Prof. Dr. A. Mielke, October 16.
5. S. Pappenguth, *Entwicklung eines Moduls zur integrierten Visualisierung numerisch berechneter Strömungsdaten mit Hilfe eines Particle-Tracing-Verfahrens* (diploma thesis), Fachhochschule für Technik und Wirtschaft Berlin, supervisor: Dr. J. Fuhrmann, January 30.

A.2 Grants[1]

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

– **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, which is coordinated by the acting head of 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)

C7: "Mean-risk optimization of electricity production in liberalized markets" (in RG 4)

C9: "Numerical simulation and control of sublimation growth of semiconductor bulk single crystals" (in RG 7)

C10: "Modelling, asymptotic analysis and numerical simulation of the dynamics of thin film nanostructures on crystal surfaces" (in RG 7)

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

C14: "Macroscopic models for precipitation in crystalline solids" (in RG 7)

C17: "Adaptive multigrid methods for local and nonlocal phase-field models of solder alloys" (in RG 7)

C18: "Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys" (in RG 1)

C21: "Reduced-order modelling and optimal control of robot guided laser material treatments" (in RG 4)

C23: "Mass conservative coupling of fluid flow and species transport in electrochemical flow cells" (in RG 3)

C26: "Storage of hydrogen in hydrides" (in RG 7)

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)

D19: "Local existence, uniqueness, and smooth dependence for quasilinear parabolic problems with non-smooth data" (in RG 1)

D20: "Pulse shaping in photonic crystal fibers" (in 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 risk" (in RG 6)

Z1.4: "Innovations in mathematics education for the engineering science" (in RG 4)

– Collaborative Research Center (SFB) 555, Humboldt-Universität zu Berlin,
"Komplexe Nichtlineare Prozesse. Analyse — Simulation — Steuerung — Optimierung" (Complex Non-linear Processes. Analysis — Simulation — Control — Optimization)

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

B2 “Analytische und numerische Untersuchungen von raum-zeitlichen Phänomenen bei gekoppelten Halbleiterlasern” (Analytical and numerical investigation of spatio-temporal phenomena in coupled semiconductor lasers; in RG 2)

– Collaborative Research Center (SFB) 649, Humboldt-Universität zu Berlin, “Ökonomisches Risiko” (Economic Risk)

  B5: “Strukturadaptive Datenanalyse” (Structural adaptive data analysis; in RG 6)

  B7: “Kalibrierungs- und Bewertungsfehler im Risikomanagement” (Calibration and pricing errors in risk management; in RG 6)

– Collaborative Research Center (SFB) 787, Technische Universität Berlin, “Halbleiter-Nanophotonik: Materialien, Modelle, Bauelemente” (Semiconductor Nanophotonics: Materials, Models, Devices)

  B4: “Multi-dimensionale Modellierung und Simulation von VCSELn” (Multidimensional modeling and simulation of VCSEL devices; in RG 1, RG 2, and RG 3)

  B5: “Effektive Modelle, Simulation und Analysis der Dynamik in Quantenpunkt-Bauelementen” (Effective models, simulation and analysis of the dynamics in quantum dot devices; in RG 2 and RG 7)

– Priority Program SPP 1095: “Analysis, Modellbildung und Simulation von Mehrskalenproblemen” (Analysis, Modeling and Simulation of Multiscale Problems) – Coordinator Program: A. Mielke (Head of RG 1)

  “Elektronische Zustände in Halbleiternanostrukturen und Upscaling auf halbklassische Modelle” (Electronic states in semiconductor nanostructures and upscaling to semi-classical models; in RG 1 and RG 3)

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

– Priority Program SPP 1164: “Nano- und Mikrofluidik: Von der molekularen Bewegung zur kontinuierlichen Strömung” (Nano- & Microfluidics: Bridging the Gap between Molecular Motion and Continuum Flow)

  “Mathematical modeling, analysis, numerical simulation of thin films and droplets on rigid and viscoelastic substrates, emphasizing the role of slippage” (in RG 7)

– Priority Program SPP 1180: “Prognose und Beeinflussung der Wechselwirkungen von Strukturen und Prozessen” (Prediction and Manipulation of Interactions 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)

– Priority Program SPP 1204: “Algorithmen zur schnellen, werkstoffgerechten Prozesskettengestaltung und -analyse in der Umformtechnik” (Algorithms for Fast, Material-specific Process-chain Design and Analysis in Metal Forming)

  “Simulation, Optimierung und Regelung von Gefügebildung und mechanischen Eigenschaften beim Warmwalzen von Mehrphasenstählen” (Simulation and control of phase transitions and mechanical properties during hot-rolling of multiphase steels; in RG 4)

– Research Unit FOR 797 “Analysis and Computation of Microstructure in Finite Plasticity”, Ruhr-Universität Bochum

  P5: “Regularisierung und Relaxierung zeitkontinuierlicher Probleme in der Plastizität” (Regularizations and relaxations of time-continuous problems in plasticity; in RG 1)

– **Normalverfahren (Individual Grants)**

"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)

"Evaluierung von Hypothesen und Entwicklung eines Referenzdatensystems zum Zustand von Waldökosystemen anhand von Langzeitdaten der Walddauerbeobachtung" (Evaluation of hypotheses and development of a reference data system for the condition of forest ecosystems by means of long-term data from forest monitoring; in RG 6)

"Pulsformung in Hohlfaserkompressoren: Simulation und Experiment" (Pulse shaping in hollow-fiber compressors: Simulation and experiment; in RG 2)

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

Leibniz-Gemeinschaft (Leibniz Association), Bonn and Berlin

– **Wettbewerbliches Verfahren "Pakt für Forschung und Innovation" (Competitive Procedure "Pact for Research and Innovation")**

"Gekoppelte Strömungsprozesse in Energie- und Umweltforschung" (Coupled flow processes in energy and environmental research, coordinator: J. Fuhrmann, RG 3)

Alexander von Humboldt-Stiftung (Alexander von Humboldt Foundation), Bonn

– A laureate of the Humboldt Research Award (in RG 2), see page 150

Deutscher Akademischer Austauschdienst (German Academic Exchange Service), Bonn

– Project-based Personnel Exchange Program with Poland (State Committee for Scientific Research, KBN): "Dynamic complexity in systems with delay" (Technical University of Łodz with RG 2)

Technologiestiftung Berlin (Technology Foundation Berlin)

– Verbundprojekt (research network project): KRIST*MAG*® (in RG 7)

– Verbundprojekt (research network project): AVANT*SOLAR* (in RG 7)

International Projects

– **EU FP7 Specific Targeted Research Project**: "Material Development for Double Exposure and Double Patterning (MD^3)", Workpackage 3 "Simulation", task "Post exposure bake in photholithography" (in RG 3)

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

– **GIF** (German-Israeli Foundation for Scientific Research & Development): "Metastability and phase segregation" (in RG 5)

– **RGI (Ruimte voor Geo-Informatie), in cooperation with the Delft University of Technology, Research Institute OTB, Section GISt**: Consortium for Program "Geo connected", in RG 3

– **SFI Research Frontiers Program 2006**: "Bifurcations in systems with hysteresis and nonsmooth nonlinearities" (in RG 2)

– A. Bovier, until October 2008 head of RG 5, was the Coordinator of the International Research Training Group GRK 1339 “Stochastic Models of Complex Systems and their Applications” (DFG/Swiss National Science Foundation).

– A. Bovier, until October 2008 head of RG 5, is also 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”.

Mission-oriented research (examples)

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

– Deutsches Elektronen-Synchrotron (German Electron Synchrotron, DESY), Hamburg: “Numerical investigation of the movement of large clouds in depleted Si detectors” (in RG 3)

– Electricité de France (EDF), Clamart: “Optimization problems with chance constraints applied to electricity portfolio” (in RG 4)

– Endress+Hauser Flowtec AG, Reinach, Switzerland: “Simulation des Verzugs beim Schweißen eines Durchflussmessergehäuses” (Simulation of distortion of a flow meter case during welding; in RG 4)

– Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin: “Mathematische Modellierung und Simulation von MOPA-Diodenlasern” (Mathematical modeling and simulation of MOPA diode lasers; in RG 2)

– Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin: “Wellenlängenstabilisierte Halbleiterlaser” (Wavelength-stabilized semiconductor lasers; in RG2)

– HSH Nordbank AG, Kiel: “Robuste Kalibrierung des erweiterten Libor-Markt-Modells” (Robust calibration of the extended Libor market model; in RG 6)

– International Intellectual Group, Inc., St. Petersburg/Staten Island: “A conical diffraction solver for multiple penetrating profiles” (in RG 4)

– Landesbank Berlin AG: “Entwicklung erweiterter Libor-Markt-Modelle, Kalibrierung, Bewertung und Replikation komplex strukturierter Produkte” (Development of expanded Libor market models, calibration, pricing, and replication of complex structured products, in RG 6)

– Physikalisch-Technische Bundesanstalt, Braunschweig and Berlin: “Vermessung von Lithographiemasken durch Scatterometrie” (Measurements of lithographic masks based on scatterometry; in RG 4)

– Rücker EKS GmbH, Weingarten: “Simulations- und Optimierungsaufgaben bei der virtuellen Fabrikplanung” (Simulation and optimal control tasks in virtual production planning”; in RG 4)

– Westdeutsche Genossenschafts-Zentralbank, Düsseldorf: “Robuste Kalibrierung des Libor-Markt-Modells” (Robust calibration of the Libor market model; in RG 6)

A.3 Membership in Editorial Boards

1. A. Bovier, Editorial Board, Electronic Communications in Probability, Institute of Mathematical Statistics (IMS) and Bernoulli Society, Nantes, France.
2. ———, Editorial Board, Electronic Journal of Probability, Institute of Mathematical Statistics (IMS) and Bernoulli Society, Nantes, France.
3. ———, Editorial Board, Markov Processes and Related Fields, Polymat, Russia.
4. M. Ehrhardt, Editorial Board, Advances in Applied Mathematics and Mechanics, Global Science Press, Wanchai, Hong Kong.
5. R. Henrion, Editorial Board, International Journal of Management Science and Engineering Management (MSEM), World Academic Press, Liverpool, UK.
6. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
7. P. Krejčí, Editor-in-Chief, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.
8. P. Mathé, Editorial Board, Journal of Complexity, Elsevier, Amsterdam, The Netherlands.
9. ———, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
10. A. Mielke, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
11. ———, Editor-in-Chief, Journal of Nonlinear Science, Springer Science+Business Media, New York, USA.
12. ———, Editor-in-Chief, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
13. ———, Co-Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
14. ———, Editorial Board, Archive for Rational Mechanics and Analysis, Springer-Verlag, Berlin, Heidelberg.
15. ———, Editorial Board, European Series in Applied and Industrial Mathematics: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
16. ———, Editorial Board, Mathematical Models and Methods in Applied Sciences, Imperial College Press, London, UK.
17. J. Polzehl, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.
18. ———, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, The Netherlands.
19. K. Sabelfeld, Editor-in-Chief, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
20. ———, Senior Editor, Mathematics and Computers in Simulation, Elsevier, Amsterdam, The Netherlands.
21. J. Sprekels, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.
22. ———, Editor, Advances in Mathematical Sciences and Applications, Gakkōtosho, Tokyo, Japan.
23. W. Wagner, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.

A.4 Conferences, Colloquia, and Workshops

A.4.1 WIAS Conferences, Colloquia, and Workshops

4th Workshop on Mathematical Models for Transport in Macroscopic and Mesoscopic Systems
Berlin, February 7–10
Organized by: WIAS (RG 1)
Supported by: DFG (SPP 1095 "Analysis, Modeling and Simulation of Multiscale Problems"), WIAS

The workshop was the fourth of a series of workshops having taken place before in Bucharest, Aalborg, and Marseille. The series is devoted to problems of electron transport in solid state physics and is interesting for mathematicians, mathematical and theoretical physicists, as well as specialists in semiconductor devices. The topic covers classical, semi-classical, and quantum models of electron transport in semiconductors. This workshop brought together 26 scientists from Europe working on electron transport in semiconductors. From the 20 talks, 14 were invited. The next workshops are planned in Dublin and Aalborg.

DFG Priority Program SPP 1180 Workshop "Parameteridentifikation bei Werkzeugmaschinen" (Parameter identification for machine tools)
Berlin, February 21–22
Organized by: WIAS (RG 4)
Supported by: DFG (SPP 1180)

The goal of this workshop was to bring together the groups of the DFG Priority Program SPP 1180 "Prediction and Manipulation of Interaction between Structure and Process" working on problems related to metal-cutting. The 33 participants discussed issues related to the identification of machine dynamics. Two additional talks gave an overview of new measurement techniques and state-of-the-art mathematical approaches to parameter identification.

Matheon–ICM Workshop on Free Boundaries and Materials Modeling
Berlin, March 17–18
Organized by: WIAS (RG 1 and RG 7), Matheon Project Group C18 "Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys"
Supported by: DFG Research Center Matheon, WIAS

The workshop took place on March 17–18 at WIAS and brought together 33 researchers, among them nine invited scientists from the *Interdisciplinary Centre for Mathematical and Computational Modelling (ICM)* in Warsaw. The lectures covered the modeling of crystal growth and of drift-diffusion phenomena, multiscale modeling and simulation of complex materials, and the mathematical and numerical analysis for multiphase and phase transformation models. The workshop was a successful first step towards a close cooperation between ICM Warsaw and Matheon/WIAS Berlin.

Workshop "Random Systems from Physics to Biology"
Berlin, March 17–20
Organized by: TU Berlin, WIAS (RG 5)
Supported by: DFG, WIAS

The Workshop "Random Systems from Physics to Biology" took place March 17–20, 2008, at the Technical University (TU) of Berlin. It was organized by Anton Bovier, Jean-Dominique Deuschel, and Jürgen Gärtner (both TU). This workshop was a joint initiative of two DFG-funded research groups, the Dutch-German Bilateral Research Group "Mathematics of Random Spatial Models from Physics and Biology" and the DFG Research Group "Analysis and Stochastics in Complex Physical Systems" (Berlin–Leipzig) and featured invited lectures by renowned international experts such as Anna de Masi, Vladas Sidoravicius, Roberto Fernandez, Mathew Penrose, Nathaniel Berestycki, Alejandro Ramirez, and Takashi Kumagai, as well as 14 talks by junior members of the two research groups. About 50 participants attended the workshop.

Workshop "Mathematics in Industry: Technologies of Thin Film Solar Cells"
Berlin, October 6–9
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", University of Nottingham, Technische Universität (TU) Berlin, Hahn–Meitner Institute (HMI), Berlin (now Helmholtz Centre Berlin for Materials and Energy (HZB))
Supported by: DFG Research Center Matheon, WIAS

The success of the first WIAS/Matheon Interdisciplinary Workshop "Mathematical Problems in Industry: Process Engineering of Thin Liquid Films" (WIAS, Juli 18–21, 2005), organized by Barbara Wagner, Andreas Münch (HU Berlin), Volker Mehrmann, and Matthias Kraume (both TU Berlin), motivated this workshop, organized by Barbara Wagner, Andreas Münch (University of Nottingham, UK), Volker Mehrmann (TU Berlin), and Bernd Rech (HZB).

The topic of this workshop reflects the growing demand for advanced technologies in the photovoltaic industry, and the growing expertise, both, on the engineering side, represented by participants from HZB (HMI), and on the theoretical side within the application areas of the DFG Research Center Matheon.

The workshop had 49 participants, largely from Germany, but also from the UK, USA, Czech Republic, and Belarus. Four companies presented their problems, all of which were intensely investigated by the teams that formed during the workshop. The goal to initiate collaboration of universities and research institutes with industry has worked for all the problems presented and it is hoped that it will lead to novel theoretical approaches to advance the photovoltaic industry.

Workshop "Phase Transitions and Optimal Control"
Berlin, October 23–25
Organized by: WIAS (RG 4 and RG 7)
Supported by: DFG

The workshop focused on three main research areas: phase transitions, optimal control, and hysteresis. The word "hysteresis" is usually attributed to processes that exhibit a rate-independent memory. The physical reason for rate independence relies on structure changes in a hidden microstructure, which are much faster than the observer's time scale. Phase transitions offer a typical example of such a behavior. Due to the lack of smoothness, optimal control of such processes represents a special challenge for mathematicians.

Seventy participants from 15 countries participated in the workshop, discussing new developments and listening to 24 invited talks in this exciting field on the interface of materials science, analysis, optimization, and numerics.

Workshop "Complex Dynamics in Large Coupled Systems"
Berlin, November 17–19
Organized by: WIAS (RG 2, Matheon Project Groups D8 "Nonlinear dynamical effects in integrated optoelectronic structures" and D21 "Synchronization phenomena in coupled dynamical systems")
Supported by: DFG (SFB 555 "Complex Nonlinear Processes"), DFG Research Center Matheon

This interdisciplinary workshop gathered physicists and mathematicians working in the fields of complex dynamics and coupled systems of different nature: optoelectroncis, neuroscience, etc. The workshop particularly focused on new interdisciplinary approaches. Special attention was also paid to the effects of symmetry and coupling topology on the dynamics.

The major topics were:

- coupled systems in optoelectronics and neuroscience
- synchronization and chaos in coupled systems
- delayed feedback control
- delay-induced dynamical effects.

The positive response to this scientific meeting was underlined by the number of 77 participants from 14 countries. The workshop included 13 invited talks (8 of them were given by scientists from abroad) and 17 contributed presentations. The full program of the workshop can be found on the web page http://www.wias-berlin.de/workshops/dynamics08.

WORKSHOP "SPARSITY AND INVERSE PROBLEMS IN STATISTICAL THEORY AND ECONOMETRICS"
Berlin, December 5–6
Organized by: WIAS (RG 6), DFG (SFB 649 "Economic Risk"), Center for Applied Statistics and Economics (C.A.S.E., Humboldt University of Berlin), Fraunhofer Institute for Computer Architecture and Software Technology (FIRST)
Supported by: DFG (SFB 649)

Data sets with a very large number of explanatory variables are becoming more and more common as features of both applications and theoretical investigations. In economical applications, for instance, the revealed preference of market players is observed, and the analyst tries to understand them by a complex model by which the players' behavior can be understood as an indirect observation. State-of-the-art statistical approaches often formulate such models as inverse problems, but the corresponding methods can suffer from the curse of dimensionality: When there are "too many" possible explanatory variables, additional regularization is needed. Inverse problem theory already offers sophisticated regularization methods for smooth models, but is just beginning to integrate sparsity concepts. For high-dimensional linear models, sparsity regularizations have proved to be a convincing way to tackle the issue both in theory and practice, but there remains a vast ground to be explored. Paralleling the statistics community are also recent advances in machine learning methodology and statistical learning theory, where the themes of sparsity and inverse problems have been intertwined.

The focus of the workshop was on the different ways to attack the question: There are many potential models to choose from, but each of them is relatively simple—each model is parameterized by many variables, most of which are zero.

The workshop was attended by 39 participants from 10 countries and included 16 invited and contributed talks.

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

1. A. Bovier, co-organizer, *Workshop on Metastability*, EURANDOM, Eindhoven, The Netherlands, January 8–11.
2. ———, organizer of the invited session "Stochastic Processes in Physics", *7th World Congress in Probability and Statistics*, jointly organized by the Department of Statistics and Applied Probability, Department of Mathematics, and Institute for Mathematical Sciences of the National University of Singapore, Singapore, July 16–19.
3. R. Henrion, member of the Program Committee, *Conference on Optimization & Practices in Industry 2008 (COPI08)*, Clamart, France, November 26–28.
4. D. Hömberg, organizer of the minisymposium "Interactions between Structure and Process in Manufacturing Systems", *The European Consortium for Mathematics in Industry (ECMI 2008)*, University College, London, UK, June 30 – July 4.
5. ———, member of the Scientific Committee, *2nd International Conference on Distortion Engineering 2008*, Bremen, September 17–19.
6. Ch. Meyer, organizer of the minisymposium "Numerical Treatment of PDE Constrained Optimization Problems C: Applications", *SIAM Conference on Optimization*, Boston, USA, May 10–13.
7. ———, organizer of the minisymposium "Optimal Control of PDEs with Pointwise State Constraints", *Annual Meeting of the Deutsche Mathematiker-Vereinigung 2008*, Friedrich-Alexander-Universität Erlangen-Nürnberg, September 15–19.
8. A. Mielke, co-organizer of the minisymposium "Advances in Variational Evolution", *5th European Congress of Mathematics*, European Mathematical Society/VU University of Amsterdam, Amsterdam, The Netherlands, July 14–18.
9. J. Sprekels, co-organizer, *Workshop "Optimal Control of Coupled Systems of PDE"*, Mathematisches Forschungsinstitut Oberwolfach, March 2–8.
10. W. Wagner, co-organizer, *Mini-workshop "Numerics for Kinetic Equations"*, Mathematisches Forschungsinstitut Oberwolfach, November 16–22.

A.6 Publications

Monographs (to appear)

[1] M. Ehrhardt, ed., *Wave Propagation in Periodic Media — Analysis, Numerical Techniques and Practical Applications*, vol. 1 of Progress in Computational Physics (PiCP), Bentham Science Publishers Ltd.

A.6.1 Editorship of Proceedings and Collected Editions

[1] M. Ehrhardt, ed., *Nonlinear Models in Mathematical Finance: New Research Trends in Option Pricing*, Nova Science Publishers, New York, USA, 2008, vii+352+8 pages.

[2] R. Henrion, A. Kruger, J. Outrata, eds., *Special Issue on: Variational Analysis and Generalised Differentiation*, vol. 16 of Set-Valued Analysis, Springer, Heidelberg, 2008, xii+231 pages.

[3] D. Hömberg, P. Krejčí, eds., *Special Issue Dedicated to Jürgen Sprekels*, vol. 53 of Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague, 2008, 115 pages.

[4] P. Colli, A. Damlamian, N. Kenmochi, M. Mimura, J. Sprekels, eds., *Proceedings of International Conference on: Nonlinear Phenomena with Energy Dissipation: Mathematical Analysis, Modeling and Simulation*, vol. 29 of Gakuto International Series Mathematical Sciences and Applications, Gakkōtosho, Tokyo, 2008, 475 pages.

A.6.2 Outstanding Contributions to Monographs

[1] W. Dreyer, *Herstellung und Einsatz moderner Materialien, in: Produktionsfaktor Mathematik. Wie Mathematik Technik und Wirtschaft bewegt*, M. Grötschel, K. Lucas, V. Mehrmann, eds., acatech diskutiert, acatech, Springer, Berlin, Heidelberg, 2008, pp. 307–322.

[2] M. Ehrhardt, *Chapter 1: Nonlinear Models in Option Pricing — An Introduction, in: Nonlinear Models in Mathematical Finance: New Research Trends in Option Pricing*, M. Ehrhardt, ed., Nova Science Publishers, New York, USA, 2008, pp. 1–19.

[3] J. Ankudinova, M. Ehrhardt, *Chapter 8: Fixed Domain Transformations and Split-step Finite Difference Schemes for Nonlinear Black–Scholes Equations for American Options, in: Nonlinear Models in Mathematical Finance: New Research Trends in Option Pricing*, M. Ehrhardt, ed., Nova Science Publishers, New York, USA, 2008, pp. 243–273.

[4] B. Denkena, D. Hömberg, E. Uhlmann, *Mathematik für Werkzeugmaschinen und Fabrikautomatisierung, in: Produktionsfaktor Mathematik. Wie Mathematik Technik und Wirtschaft bewegt*, M. Grötschel, K. Lucas, V. Mehrmann, eds., acatech diskutiert, acatech, Springer, Berlin, Heidelberg, 2008, pp. 279–299.

[5] I. Laukaityte, R. Čiegis, M. Lichtner, M. Radziunas, *Parallel Numerical Algorithm for the Traveling Wave Model, in: Parallel Scientific Computing and Optimization: Advances and Applications*, R. Čiegis, D. Henty, B. Kågström, J. Žilinskas, eds., vol. 27 of Springer Optimization and Its Applications, Springer, New York, 2008, pp. 237–251.

[6] M. Tlidi, R. Lefever, A.G. Vladimirov, *On Vegetation Clustering, Localized Bare Soil Spots and Fairy Circles, in: Dissipative Solitons: From Optics to Biology and Medicine*, N. Akhmediev, A. Ankiewicz, eds., vol. 751 of Lecture Notes in Physics, Springer, Berlin, Heidelberg, 2008, pp. 381–402.

Contributions to Monographs (to appear)

[1] A. Arnold, M. Ehrhardt, M. Schulte, *Chapter 6: Numerical Simulation of Quantum Waveguides, in: VLSI and Computer Architecture*, K. Watanabe, ed., Nova Science Publishers, New York, USA.

A.6.3 Articles in Refereed Journals[2]

[1] K. Afanasiev, A. Münch, B. Wagner, *Thin film dynamics on a vertically rotating disk partially immersed in a liquid bath*, Appl. Math. Modelling, 32 (2008), pp. 1894–1911.

[2] S. Amiranashvili, A.G. Vladimirov, U. Bandelow, *Solitary-wave solutions for few-cycle optical pulses*, Phys. Rev. A, 77 (2008), pp. 063821/1–063821/7.

[3] M. Birkner, *Conditional large deviations for a sequence of words*, Stochastic Process. Appl., 118 (2008), pp. 703–729.

[4] M. Birkner, J. Blath, *Computing likelihoods for coalescents with multiple collisions in the infinitely-many-sites model*, J. Math. Biol., 57 (2008), pp. 435–465.

[5] G. Ben Arous, A. Bovier, J. Černý, *Universality of the REM for dynamics of mean field spin glasses*, Comm. Math. Phys., 282 (2008), pp. 633–695.

[6] ———, *Universality of the REM-like ageing in mean field spin glasses*, J. Stat. Mech. Theory Exp., 4 (2008), pp. L04003/1–L04003/8.

[7] A. Bovier, A. Faggionato, *Spectral analysis of Sinai's random walk*, Ann. Probab., 36 (2008), pp. 198–254.

[8] A. Bovier, A. Klimovski, *Fluctuations of the partition function in the GREM with external field*, J. Math. Phys., 49 (2008), pp. 125202/1–125202/22.

[9] A. Demircan, M. Pietrzyk, U. Bandelow, *Effects of higher-order dispersion on pulse splitting in the normal dispersion regime*, Opt. Quantum Electron., 40 (2008), pp. 455–460.

[10] W. Dreyer, M. Herrmann, *Numerical experiments on the modulation theory for the nonlinear atomic chain*, Phys. D, 237 (2008), pp. 255–282.

[11] W. Dreyer, F. Duderstadt, *On the modelling of semi-insulating GaAs including surface tension and bulk stresses*, Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci., 464 (2008), pp. 2693–2720.

[12] P.-E. Druet, *Weak solutions to a stationary heat equation with nonlocal radiation boundary condition and right-hand side in L^p with $p \geq 1$*, Math. Methods Appl. Sci., 32 (2008), pp. 135–166.

[13] M. Ehrhardt, *Discrete transparent boundary conditions for Schrödinger-type equations for non-compactly supported initial data*, Appl. Numer. Math., 58 (2008), pp. 660–673.

[14] X. Antoine, A. Arnold, Ch. Besse, M. Ehrhardt, A. Schädle, *A review of transparent and artificial boundary conditions techniques for linear and nonlinear Schrödinger equations*, Commun. Comput. Phys., 4 (2008), pp. 729–796.

[15] A. Bratsos, M. Ehrhardt, I.T. Famelis, *A discrete Adomian decomposition method for discrete nonlinear Schrödinger equations*, Appl. Math. Comput., 197 (2008), pp. 190–205.

[16] M. Ehrhardt, R. Mickens, *Discrete models for the cube-root differential equation*, Neural Parallel Sci. Comput., 16 (2008), pp. 179–188.

[17] ———, *A fast, stable and accurate numerical method for the Black–Scholes equation of American options*, Int. J. Theor. Appl. Finance, 11 (2008), pp. 471–501.

[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.

[18] M. Ehrhardt, Ch. Zheng, *Exact artificial boundary conditions for problems with periodic structures*, J. Comput. Phys., 227 (2008), pp. 6877–6894.

[19] J. Ankudinova, M. Ehrhardt, *On the numerical solution of nonlinear Black–Scholes equations*, Comput. Math. Appl., 56 (2008), pp. 799–812.

[20] A. Zisowsky, M. Ehrhardt, *Discrete artificial boundary conditions for nonlinear Schrödinger equations*, Math. Comput. Modelling, 47 (2008), pp. 1264–1283.

[21] J. Elschner, M. Yamamoto, *Uniqueness in determining polyhedral sound-hard obstacles with a single incoming wave*, Inverse Problems, 24 (2008), pp. 035004/1–035004/7.

[22] J. Elschner, G. Hsiao, A. Rathsfeld, *An inverse problem for fluid-solid interaction*, Inverse Probl. Imaging, 2 (2008), pp. 83–120.

[23] P. Ferrari, *Slow decorrelations in Kardar–Parisi–Zhang growth*, J. Stat. Mech. Theory Exp., (2008), pp. P07022/1–P07022/18.

[24] F. Bornemann, P. Ferrari, M. Prähofer, *The Airy$_1$ process is not the limit of the largest eigenvalue in GOE matrix diffusion*, J. Statist. Phys., 133 (2008), pp. 405–415.

[25] A. Borodin, P. Ferrari, T. Sasamoto, *Large time asymptotics of growth models on space-like paths II: PNG and parallel TASEP*, Comm. Math. Phys., 283 (2008), pp. 417–449.

[26] A. Borodin, P. Ferrari, *Large time asymptotics of growth models on space-like paths I: PushASEP*, Electron. J. Probab., 13 (2008), pp. 1380–1418.

[27] J. Fuhrmann, H. Zhao, E. Holzbecher, H. Langmach, *Flow, transport, and reactions in a thin layer flow cell*, J. Fuel Cell Sci. Techn., 5 (2008), pp. 021008/1–021008/10.

[28] J. Fuhrmann, H. Zhao, E. Holzbecher, H. Langmach, M. Chojak, R. Halseid, Z. Jusys, R. Behm, *Experimental and numerical model study of the limiting current in a channel flow cell with a circular electrode*, Phys. Chem. Chem. Phys., 10 (2008), pp. 3784–3795.

[29] A. Glitzky, *Analysis of a spin-polarized drift-diffusion model*, Adv. Math. Sci. Appl., 18 (2008), pp. 401–427.

[30] ———, *Exponential decay of the free energy for discretized electro-reaction-diffusion systems*, Nonlinearity, 21 (2008), pp. 1989–2009.

[31] A. Glitzky, R. Hünlich, *Stationary solutions to an energy model for semiconductor devices where the equations are defined on different domains*, Math. Nachr., 281 (2008), pp. 1676–1693.

[32] J.A. Griepentrog, W. Höppner, H.-Chr. Kaiser, J. Rehberg, *A bi-Lipschitz continuous, volume preserving map from the unit ball onto a cube*, Note Mat., 28 (2008), pp. 185–201.

[33] S. Heinz, *Quasiconvex functions can be approximated by quasiconvex polynomials*, ESAIM Control Optim. Calc. Var., 14 (2008), pp. 795–801.

[34] R. Henrion, Ch. Küchler, W. Römisch, *Discrepancy distances and scenario reduction in two-stage stochastic integer programming*, J. Indust. Management Optim., 4 (2008), pp. 363–384.

[35] R. Henrion, J. Outrata, *On calculating the normal cone to a finite union of convex polyhedra*, Optimization, 57 (2008), pp. 57–78.

[36] R. Henrion, A. Seeger, *Uniform boundedness of norms of convex and nonconvex processes*, Numer. Funct. Anal. Optim., 29 (2008), pp. 551–573.

[37] R. Henrion, C. Strugarek, *Convexity of chance constraints with independent random variables*, Comput. Optim. Appl., 41 (2008), pp. 263–276.

[38] H. Cornean, K. Hoke, H. Neidhardt, P.N. Racec, J. Rehberg, *A Kohn–Sham system at zero temperature*, J. Phys. A, 41 (2008), pp. 385304/1–385304/21.

[39] K. Chełminski, D. Hömberg, D. Kern, *On a thermomechanical model of phase transitions in steel*, Adv. Math. Sci. Appl., 18 (2008), pp. 119–140.

[40] R. Haller-Dintelmann, H.-Chr. Kaiser, J. Rehberg, *Elliptic model problems including mixed boundary conditions and material heterogeneities*, J. Math. Pures Appl., 89 (2008), pp. 25–48.

[41] J. Kampen, A. Kolodko, J.G.M. Schoenmakers, *Monte Carlo Greeks for financial products via approximative transition densities*, SIAM J. Sci. Comput., 31 (2008), pp. 1–22.

[42] J. Geiser, O. Klein, P. Philip, *A finite volume scheme designed for anisotropic heat transfer in general polyhedral domains*, Adv. Math. Sci. Appl., 18 (2008), pp. 43–67.

[43] M. Eleuteri, O. Klein, P. Krejčí, *Outward pointing inverse Preisach operators*, Phys. B, 403 (2008), pp. 254–256.

[44] O. Klein, Ch. Lechner, P.-E. Druet, P. Philip, J. Sprekels, Ch. Frank-Rotsch, F.M. Kiessling, W. Miller, U. Rehse, P. Rudolph, *Numerical simulation of Czochralski crystal growth under the influence of a traveling magnetic field generated by an internal heater-magnet module (HMM)*, J. Crystal Growth, 310 (2008), pp. 1523–1532.

[45] D. Knees, *Global stress regularity of convex and some nonconvex variational problems*, Ann. Mat. Pura Appl. IV. Ser., 187 (2008), pp. 157–184.

[46] D. Knees, P. Neff, *Regularity up to the boundary for nonlinear elliptic systems arising in time-incremental infinitesimal elasto-plasticity*, SIAM J. Math. Anal., 40 (2008), pp. 21–43.

[47] D. Knees, A. Mielke, *Energy release rate for cracks in finite-strain elasticity*, Math. Methods Appl. Sci., 31 (2008), pp. 501–528.

[48] ———, *On the energy release rate in finite-strain elasticity*, Mech. Adv. Mater. Struct., 15 (2008), pp. 421–427.

[49] D. Knees, A. Mielke, Ch. Zanini, *On the inviscid limit of a model for crack propagation*, Math. Models Methods Appl. Sci., 18 (2008), pp. 1529–1569.

[50] Ch. Bender, A. Kolodko, J.G.M. Schoenmakers, *Enhanced policy iteration for American options via scenario selection*, Quant. Finance, 8 (2008), pp. 135–146.

[51] M.D. Korzec, P.L. Evans, A. Münch, B. Wagner, *Stationary solutions of driven fourth- and sixth-order Cahn–Hilliard type equations*, SIAM J. Appl. Math., 69 (2008), pp. 348–374.

[52] Ch. Kraus, *Multivariate polynomial approximation of powers of the Euclidean distance function*, Constr. Approx., 27 (2008), pp. 323–327.

[53] P. Krejčí, *A higher order energy bound in a singular Preisach circuit*, Phys. B, 403 (2008), pp. 297–300.

[54] P. Krejčí, K. Kuhnen, *Existence, uniqueness and L_∞ -stability of the Prandtl–Ishlinskii hysteresis and creep compensator*, Eur. J. Control, 14 (2008), pp. 409–417.

[55] M. Brokate, M. Eleuteri, P. Krejčí, *On a model for electromagnetic processes inside and outside a ferromagnetic body*, Math. Methods Appl. Sci., 31 (2008), pp. 1545–1567.

[56] M. Eleuteri, J. Kopfová, P. Krejčí, *On a model with hysteresis arising in magnetohydrodynamics*, Phys. B, 403 (2008), pp. 448–450.

[57] P. Krejčí, J. Sprekels, *Clamped elastic-ideally plastic beams and Prandtl–Ishlinskii hysteresis operators*, Discrete Contin. Dyn. Syst. Ser. S, 1 (2008), pp. 283–292.

[58] R.B. Guenther, P. Krejčí, J. Sprekels, *Small strain oscillations of an elastoplastic Kirchhoff plate*, ZAMM Z. Angew. Math. Mech., 88 (2008), pp. 199–217.

[59] M.C. Babiuc, S. Husa, D. Alic, I. Hinder, Ch. Lechner, E. Schnetter, B. Szilagyi, Y. Zlochower, N. Dorband, D. Pollney, J. Winicour, *Implementation of standard testbeds for numerical relativity*, Classical Quantum Gravity, 25 (2008), pp. 125012/1–125012/38.

[60] M. Lichtner, *Spectral mapping theorem for linear hyperbolic systems*, Proc. Amer. Math. Soc., 136 (2008), pp. 2091–2101.

[61] A. Linke, G. Matthies, L. Tobiska, *Non-nested multi-grid solvers for mixed divergence-free Scott–Vogelius discretizations*, Computing, 83 (2008), pp. 87–107.

[62] E. Burman, A. Linke, *Stabilized finite element schemes for incompressible flow using Scott–Vogelius elements*, Appl. Numer. Math., 58 (2008), pp. 1704–1719.

[63] P. Mathé, B. Hofmann, *Direct and inverse results in variable Hilbert scales*, J. Approx. Theory, 154 (2008), pp. 77–89.

[64] ———, *How general are general source conditions?*, Inverse Problems, 24 (2008), pp. 015009/1–015009/5.

[65] B. Hofmann, P. Mathé, M. Schieck, *Modulus of continuity for conditionally stable ill-posed problems in Hilbert space*, J. Inverse Ill-Posed Probl., 16 (2008), pp. 567–585.

[66] P. Mathé, N. Schöne, *Regularization by projection in variable Hilbert scales*, Appl. Anal., 2 (2008), pp. 201– 219.

[67] R. Krämer, P. Mathé, *Modulus of continuity of Nemytskiĭ operators with application to a problem of option pricing*, J. Inverse Ill-Posed Probl., 16 (2008), pp. 435–461.

[68] Ch. Meyer, *Error estimates for the finite element approximation of an elliptic control problem with pointwise state and control constraints*, Control Cybernet., 37 (2008), pp. 51–85.

[69] A. Mielke, *Weak-convergence methods for Hamiltonian multiscale problems*, Discrete Contin. Dyn. Syst., 20 (2008), pp. 53–79.

[70] F. Auricchio, A. Mielke, U. Stefanelli, *A rate-independent model for the isothermal quasi-static evolution of shape-memory materials*, Math. Methods Appl. Sci., 18 (2008), pp. 125–164.

[71] J. Giannoulis, A. Mielke, Ch. Sparber, *Interaction of modulated pulses in the nonlinear Schrödinger equation with periodic potential*, J. Differential Equations, 245 (2008), pp. 939–963.

[72] A. Mielke, M. Ortiz, *A class of minimum principles for characterizing the trajectories and the relaxation of dissipative systems*, ESAIM Control Optim. Calc. Var., 14 (2008), pp. 494–516.

[73] R. Rossi, A. Mielke, G. Savaré, *A metric approach to a class of doubly nonlinear evolution equations and applications*, Ann. Sc. Norm. Super. Pisa Cl. Sci. (5), VII (2008), pp. 97–169.

[74] A. Mielke, T. Roubíček, U. Stefanelli, Γ*-limits and relaxations for rate-independent evolutionary problems*, Calc. Var. Partial Differ. Equ., 31 (2008), pp. 387–416.

[75] A. Mielke, U. Stefanelli, *A discrete variational principle for rate-independent evolution*, Adv. Calculus Variations, 1 (2008), pp. 399–431.

[76] J. Giannoulis, M. Herrmann, A. Mielke, *Lagrangian and Hamiltonian two-scale reduction*, J. Math. Phys., 49 (2008), pp. 103505/1–103505/42.

[77] A. Mielke, A. Petrov, J.A.C. Martins, *Convergence of solutions of kinetic variational inequalities in the rate-independent quasi-static limit*, J. Math. Anal. Appl., 348 (2008), pp. 1012–1020.

[78] H.-G. Bartel, H.-J. Mucha, J. Dolata, *Über Identifikationsmethoden, dargestellt am Beispiel römischer Baukeramik*, Berliner Beiträge zur Archäometrie, 21 (2008), pp. 115–132.

[79] J. Behrndt, M.M. Malamud, H. Neidhardt, *Scattering matrices and Weyl functions*, Proc. London Math. Soc. (3), 97 (2008), pp. 568–598.

[80] J. Behrndt, H. Neidhardt, R. Racec, P.N. Racec, U. Wulf, *On Eisenbud's and Wigner's R-matrix: A general approach*, J. Differential Equations, 244 (2008), pp. 2545–2577.

[81] J.A. Martins, M.D. Monteiro Marques, A. Petrov, *On the stability of elastic-plastic systems with hardening*, J. Math. Anal. Appl., 343 (2008), pp. 1007–1021.

[82] A. Bhattacherjee, M. Pietrzyk, *Transport behaviour of a Bose–Einstein condensate in a bichromatic optical lattice*, Cent. Eur. J. Math., 6 (2008), pp. 26–32.

[83] M. Pietrzyk, I. Kanattšikow, U. Bandelow, *On the propagation of vector ultra-short pulses*, J. Nonlinear Math. Phys., 15 (2008), pp. 162–170.

[84] D. Divine, J. Polzehl, F. Godtliebsen, *A propagation-separation approach to estimate the autocorrelation in a time-series*, Nonlin. Processes Geophys., 15 (2008), pp. 591–599.

[85] R. Čiegis, M. Radziunas, M. Lichtner, *Numerical algorithms for simulation of multisection lasers by using traveling wave model*, Math. Model. Anal., 13 (2008), pp. 327–348.

[86] D. Turaev, M. Radziunas, A.G. Vladimirov, *Chaotic soliton walk in periodically modulated media*, Phys. Rev. E, 77 (2008), pp. 06520/1–06520/4.

[87] H. Gross, A. Rathsfeld, *Sensitivity analysis for indirect measurement in scatterometry and the reconstruction of periodic grating structures*, Waves Random Complex Media, 18 (2008), pp. 129–149.

[88] J.C. de Los Reyes, P. Merino, J. Rehberg, F. Tröltzsch, *Optimality conditions for state-constrained PDE control problems with finite-dimensional control space*, Control Cybernet., 37 (2008), pp. 7–38.

[89] R. Haller-Dintelmann, M. Hieber, J. Rehberg, *Irreducibility and mixed boundary conditions*, Positivity, 12 (2008), pp. 83–91.

[90] M. Hieber, J. Rehberg, *Quasilinear parabolic systems with mixed boundary conditions on nonsmooth domains*, SIAM J. Math. Anal., 40 (2008), pp. 292–305.

[91] A. Rohde, *Adaptive goodness-of-fit tests based on signed ranks*, Ann. Statist., 36 (2008), pp. 1346–1374.

[92] K. Sabelfeld, *Expansion of random boundary excitations for the fractional Laplacian*, J. Cosmol. Astropart. Phys., 2008 (2008), pp. 1475–7516.

[93] ———, *Stokes flows under random boundary velocity excitations*, J. Statist. Phys., 133 (2008), pp. 1107–1136.

[94] K. Sabelfeld, I. Shalimova, *Elastic half-plane under random displacement excitations on the boundary*, J. Statist. Phys., 132 (2008), pp. 1071–1095.

[95] N. Suciu, C. Vamos, H. Vereecken, K. Sabelfeld, P. Knabner, *Memory effects induced by dependence on initial conditions and ergodicity of transport in heterogeneous media*, Water Resour. Res., 44 (2008), pp. 1–26.

[96] T. Vesala, N. Kljun, U. Rannik, J. Rinne, A. Sogachev, T. Markkanen, K. Sabelfeld, Th. Foken, M. Leclerc, *Flux and concentration footprint modelling: State of the art*, Environ. Pollution, 152 (2008), pp. 653–666.

[97] O. Kurbanmuradov, K. Sabelfeld, *Convergence of Fourier-wavelet models for Gaussian random processes*, SIAM J. Numer. Anal., 46 (2008), pp. 3084–3112.

[98] F. Lanzara, V. Maz'ya, G. Schmidt, *Approximate approximations with data on a perturbed uniform grid*, Z. Anal. Anwendungen, 27 (2008), pp. 323–338.

[99] ———, *Approximate Hermite quasi-interpolation*, Appl. Anal., 87 (2008), pp. 805–827.

[100] R. Rossi, A. Segatti, U. Stefanelli, *Attractor for gradient flows of non convex potentials and applications*, Arch. Ration. Mech. Anal., 187 (2008), pp. 91–136.

[101] P. Colli, A. Segatti, *Uniform attractors for a phase transition model coupling momentum balance and phase dynamics*, Discrete Contin. Dyn. Syst., 22 (2008), pp. 909–932.

[102] G. Schimperna, A. Segatti, *Attractors for the semiflow associated with a class of doubly nonlinear parabolic equations*, Asymptot. Anal., 56 (2008), pp. 61–86.

[103] H. Si, *Adaptive tetrahedral mesh generation by constrained Delaunay refinement*, Internat. J. Numer. Methods Engrg., 75 (2008), pp. 856–880.

[104] A. Dalalyan, A. Juditsky, V. Spokoiny, *A new algorithm for estimating the effective dimension-reduction subspace*, J. Mach. Learn. Res., 9 (2008), pp. 1647–1678.

[105] I.G. Grama, V. Spokoiny, *Statistics of extremes by oracle estimation*, Ann. Statist., 36 (2008), pp. 1619–1648.

[106] V. Katkovnik, V. Spokoiny, *Spatially adaptive estimation via fitted local likelihood techniques*, IEEE Trans. Signal Process., 56 (2008), pp. 873–886.

[107] Y. Bavafa-Toosi, Ch. Blendinger, V. Mehrmann, A. Steinbrecher, R. Unger, *A new methodology for modeling, analysis, synthesis, and simulation of time-optimal train traffic in large networks*, IEEE Trans. Autom. Sci. Eng., 5 (2008), pp. 43–52.

[108] H. Stephan, A. Khrabustovskyi, *Positivity and time behavior of a linear reaction-diffusion system, non-local in space and time*, Math. Methods Appl. Sci., 31 (2008), pp. 1809–1834.

[109] K. Tabelow, J. Polzehl, A.M. Uluğ, J.P. Dyke, R. Watts, L.A. Heier, H.U. Voss, *Accurate localization of brain activity in presurgical fMRI by structure adaptive smoothing*, IEEE Trans. Med. Imaging, 27 (2008), pp. 531–537.

[110] K. Tabelow, J. Polzehl, V. Spokoiny, H.U. Voss, *Diffusion tensor imaging: Structural adaptive smoothing*, NeuroImage, 39 (2008), pp. 1763–1773.

[111] P. Suwanpinij, N. Togobytska, Ch. Keul, W. Weiss, U. Prahl, D. Hömberg, W. Bleck, *Phase transformation modeling and parameter identification from dilatometric investigations*, Steel Res. Int., 79 (2008), pp. 793–799.

[112] V.Z. Tronciu, *Excitability and coherence resonance of DFB laser with passive dispersive reflector*, Moldavian J. Phys. Sci., 7 (2008), pp. 218–223.

[113] V.Z. Tronciu, I.V. Ermakov, P. Colet, C.R. Mirasso, *Chaotic dynamics of a semiconductor laser with double cavity feedback: Applications to phase shift keying modulation*, Opt. Commun., 281 (2008), pp. 4747–4752.

[114] V.Z. Tronciu, C.R. Mirasso, P. Colet, *Chaos-based communications using on-off phase shift keying method*, Moldavian J. Phys. Sci., 7 (2008), pp. 343–349.

[115] ———, *Chaos-based communications using semiconductor lasers subject to feedback from an integrated double cavity*, J. Phys. B, 41 (2008), pp. 155401/1–155401/8.

[116] A. Münch, B. Wagner, *Galerkin method for feedback controlled Rayleigh–Bénard convection*, Nonlinearity, 21 (2008), pp. 2625–2651.

[117] M. Rauscher, R. Blossey, A. Münch, B. Wagner, *Spinodal dewetting of thin films with large interfacial slip: Implications from the dispersion relation*, Langmuir, 24 (2008), pp. 12290–12294.

[118] W. Wagner, *Deviational particle Monte Carlo for the Boltzmann equation*, Monte Carlo Methods Appl., 14 (2008), pp. 191–268.

[119] S. Yanchuk, K.R. Schneider, O. Lykova, *Amplitude synchronization in a system of two coupled semiconductor lasers*, Ukrainian Math. J., 60 (2008), pp. 426–435.

[120] S. Yanchuk, M. Wolfrum, *Destabilization patterns in large regular networks*, Phys. Rev. E, 77 (2008), pp. 026212/1–026212/7.

Articles in Refereed Journals (to appear)

[1] L.-P. Arguin, *On the structure of quasi-stationary competing particle systems*, Ann. Probab.

[2] D. Belomestny, L. Rüschendorf, M. Urusov, *Optimal stopping of integral functionals and a "no-loss" free boundary formulation*, SIAM J. Theory Probab. Appl.

[3] D. Belomestny, Ch. Bender, J.G.M. Schoenmakers, *True upper bounds for Bermudan products via non-nested Monte Carlo*, Math. Finance.

[4] D. Belomestny, G.N. Milstein, V. Spokoiny, *Regression methods in pricing American and Bermudan options using consumption processes*, Quant. Finance.

[5] A. Bianchi, *Glauber dynamics on nonamenable graphs: Boundary conditions and mixing time*, Electron. J. Probab.

[6] C. Bréé, A. Demircan, G. Steinmeyer, *Asymptotic pulse shapes in filamentary propagation of intense femtosecond pulses*, Laser Physics.

[7] P.-E. Druet, *Weak solution to time-dependent MHD equations coupled to heat transfer with nonlocal radiation boundary conditions*, Nonlinear Anal. Real World Appl.

[8] O. Gloger, M. Ehrhardt, Th. Dietrich, O. Hellwich, K. Graf, E. Nagel, *A threestepped coordinated level set segmentation method for identifying atherosclerotic plaques on MR images*, Comm. Numer. Methods Engrg.

[9] M. Ehrhardt, H. Han, Ch. Zheng, *Numerical simulation of waves in periodic structures*, Commun. Comput. Phys.

[10] J. Fuhrmann, A. Erdmann, Ch.R. Szmanda, A. Fiebach, M. Uhle, *A model of self-limiting residual acid diffusion for pattern doubling*, Microelectronic Engineering.

[11] K. Gärtner, *Existence of bounded discrete steady state solutions of the van Roosbroeck system on boundary conforming Delaunay grids*, SIAM J. Sci. Comput.

[12] E. Giacomini, W. Härdle, V. Spokoiny, *Inhomogeneous dependency modelling with time varying copulae*, J. Bus. Econom. Statist.

[13] A. Glitzky, *Energy estimates for electro-reaction-diffusion systems with partly fast kinetics*, Discrete Contin. Dyn. Syst.

[14] A. Glitzky, K. Gärtner, *Energy estimates for continuous and discretized electro-reaction-diffusion systems*, Nonlinear Anal.

[15] R. Henrion, Ch. Küchler, W. Römisch, *Scenario reduction in stochastic programming with respect to discrepancy distances*, Comput. Optim. Appl.

[16] R. Henrion, J. Outrata, Th. Surowiec, *On the co-derivative of normal cone mappings to inequality systems*, Nonlinear Anal.

[17] R. Henrion, W. Römisch, *Lipschitz and differentiability properties of quasi-concave and singular normal distribution functions*, Ann. Oper. Res.

[18] E. Holzbecher, C. Kohfahl, *The use of COMSOL in teaching groundwater flow and transport*, Internat. J. Engrg. Education.

[19] E. Holzbecher, S. Kühn, H. Kerndorff, *A simple method to check for natural attenuation downstream of abandoned waste disposal facilities*, Internat. J. Environment Pollution.

[20] A. Fasano, D. Hömberg, L. Panizzi, *A mathematical model for case hardening of steel*, Math. Models Methods Appl. Sci.

[21] D. Hömberg, N. Togobytska, M. Yamamoto, *On the evaluation of dilatometer experiments*, Appl. Anal.

[22] H.-Chr. Kaiser, H. Neidhardt, J. Rehberg, *Classical solutions of drift-diffusion equations for semiconductor devices: The 2D case*, Nonlinear Anal.

[23] ———, *Monotonicity properties of the quantum mechanical particle density: An elementary proof*, Monatsh. Math.

[24] L. Göllmann, D. Kern, H. Maurer, *Optimal control problems with delays in state and control and mixed control-state constraints*, Optimal Control Appl. Methods.

[25] K. Kuhnen, P. Krejčí, *Compensation of complex hysteresis and creep effects in piezoelectrically actuated systems — A new Preisach modeling approach*, IEEE Trans. Autom. Control.

[26] M. Lichtner, *Variation of constants formula for hyperbolic systems*, J. Appl. Anal.

[27] M. Spreemann, M. Lichtner, M. Radziunas, U. Bandelow, H. Wenzel, *Measurement and simulation of distributed-feedback tapered master-oscillator power-amplifiers*, IEEE J. Quantum Electron.

[28] J. Härdtlein, C. Pflaum, A. Linke, C.H. Wolters, *Advanced expression templates programming*, Comput. Vis. Sci.

[29] P. Mathé, S.V. Pereverzev, *The use of higher order finite difference schemes is not dangerous*, J. Complexity.

[30] Ch. Meyer, I. Yousept, *Regularization of state-constrained elliptic optimal control problems with nonlocal radiation interface conditions*, Comput. Optim. Appl.

[31] ———, *State-constrained optimal control of semilinear elliptic equations with nonlocal radiation interface conditions*, SIAM J. Control Optim.

[32] M. Hinze, Ch. Meyer, *Numerical analysis of Lavrentiev-regularized state constrained elliptic control problems*, Comput. Optim. Appl.

[33] G. Bouchitté, A. Mielke, T. Roubíček, *A complete-damage problem at small strains*, Z. Angew. Math. Phys.

[34] A. Mielke, F. Rindler, *Reverse approximation of energetic solutions to rate-independent processes*, NoDEA Nonlinear Differential Equations Appl.

[35] A. Mielke, R. Rossi, G. Savaré, *Modeling solutions with jumps for rate-independent systems on metric spaces*, Discrete Contin. Dyn. Syst.

[36] A. Mainik, A. Mielke, *Global existence for rate-independent gradient plasticity at finite strain*, J. Nonlinear Sci.

[37] S. Zelik, A. Mielke, *Multi-pulse evolution and space-time chaos in dissipative systems*, Mem. Amer. Math. Soc.

[38] H.D. Cornean, H. Neidhardt, V.A. Zagrebnov, *The effect of time-dependent coupling on non-equilibrium steady states*, Ann. Henri Poincare.

[39] H. Neidhardt, V.A. Zagrebnov, *Linear non-autonomous Cauchy problems and evolution semigroups*, Adv. Differential Equations.

[40] A. Petrov, M. Schatzman, *Mathematical results on existence for viscoelastodynamic problems with unilateral constraints*, SIAM J. Math. Anal.

[41] J. Polzehl, S. Sperlich, *A note on structural adaptive dimension reduction*, J. Stat. Comput. Simul.

[42] K. Sabelfeld, I. Shalimova, A.I. Levykin, *Stochastic simulation method for a 2D elasticity problem with random loads*, Probab. Eng. Mech.

[43] G. Schmidt, *Integral equations for conical diffraction by coated gratings*, J. Integral Equations Appl.

[44] V. Spokoiny, *Multiscale local change point detection with applications to Value-at-Risk*, Ann. Statist.

[45] V. Spokoiny, C. Vial, *Parameter tuning in pointwise adaptation using a propagation approach*, Ann. Statist.

[46] J. Sprekels, D. Tiba, *The control variational approach for differential systems*, SIAM J. Control Optim.

[47] H. Stephan, *Modeling of drift-diffusion systems*, ZAMP Z. Angew. Math. Phys.

[48] K. Tabelow, V. Piëch, J. Polzehl, H.U. Voss, *High-resolution fMRI: Overcoming the signal-to-noise problem*, J. Neurosci. Meth.

[49] J.R. King, A. Münch, B. Wagner, *Linear stability analysis of a sharp-interface model for dewetting thin films*, J. Engrg. Math.

[50] G. Kitavtsev, B. Wagner, *Coarsening dynamics of slipping droplets*, J. Engrg. Math.

[51] A. Weiss, *Escaping the Brownian stalkers*, Electron. J. Probab.

A.6.4 Contributions to Collected Editions

[1] W. Dreyer, *From the global entropy inequality to kinetic relations*, in: Hyperbolic Aspects of Phase Transition Dynamics, Mini-workshop, February 24 – March 1, 2008, vol. 5 of Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach, 2008, pp. 532–535.

[2] P.-E. Druet, *Weak solutions to a model for global heat transfer arising in crystal growth from the melt with applied magnetic fields*, in: Optimal Control of Coupled Systems of PDE, Workshop, March 2–8, 2008, vol. 5 of Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach, 2008, pp. 597–599.

[3] M. Ehrhardt, J. Fuhrmann, A. Linke, E. Holzbecher, *Mathematical modeling of channel-porous layer interfaces in PEM fuel cells*, in: Proceedings of FDFC2008 — Fundamentals and Developments of Fuel Cell Conference 2008, Nancy, France, December 10–12 (CD), 2008, 8 pages.

[4] M. Elagin, V. Spokoiny, *Locally time homogeneous time series modelling*, in: Applied Quantitative Finance (2nd edition), W. Härdle, N. Hautsch, L. Overbeck, eds., Springer, Berlin, 2008, pp. 345–362.

[5] J. Elschner, G.C. Hsiao, A. Rathsfeld, *Direct and inverse problems in fluid-solid interaction*, in: Analysis of Boundary Element Methods, Workshop, April 14–18, 2008, M. Costabel, E.P. Stephan, eds., vol. 5 of Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach, 2008, pp. 1023–1025.

[6] H. Gajewski, J.A. Griepentrog, A. Mielke, J. Beuthan, U. Zabarylo, O. Minet, *Image segmentation for the investigation of scattered-light images when laser-optically diagnosing rheumatoid arthritis*, in: Mathematics – Key Technology for the Future, W. Jäger, H.-J. Krebs, eds., Springer, Heidelberg, 2008, pp. 149–161.

[7] D. Hömberg, D. Kern, *The heat treatment of steel — A mathematical control problem*, in: Proceedings of the 2nd International Conference on Distortion Engineering – IDE 2008, 17–19 September 2008, Bremen, Germany, H.-W. Zoch, T. Lübben, eds., IWT, Bremen, 2008, pp. 201–209.

[8] J. Kampen, *On optimal strategies of multivariate passport options*, in: Progress in Industrial Mathematics at ECMI 2006, L.L. Bonilla, M. Moscoso, G. Platero, J.M. Vega, eds., vol. 12 of Mathematics in Industry, Springer, Berlin, Heidelberg, 2008, pp. 666–670.

[9] C. Croitoru, Ch. Fries, W. Jäger, J. Kampen, D.-J. Nonnenmacher, *On the dynamics of the forward interest rate curve and the evaluation of interest rate derivatives and their sensitivities*, in: Mathematics — Key Technology for the Future, W. Jäger, H.-J. Krebs, eds., Springer, Heidelberg, 2008, pp. 343–357.

[10] O. Klein, *Outward pointing properties for vectorial hysteresis operators and some applications*, in: International Workshop on Multi-Rate Processes and Hysteresis", March 31 – April 5, 2008, Cork, Ireland, vol. 138 of J. Phys.: Conf. Ser., Inst. Phys., 2008, pp. 012009/1–012009/14.

[11] O. Klein, P.-E. Druet, J. Sprekels, Ch. Lechner, P. Philip, Ch. Frank-Rotsch, F.-M. Kiessling, W. Miller, U. Rehse, P. Rudolph, *Numerical simulations of the influence of a traveling magnetic field, generated by an internal heater magnetic module, on Czochralski crystal growth*, in: Proceedings of the International Scientific Colloquium Modelling for Electromagnetic Processing (MEP2008), Hannover, October 26–29, 2008, E. Braake, B. Nacke, eds., Leibniz University of Hannover, 2008, pp. 91–96.

[12] P. Rudolph, Ch. Frank-Rotsch, F.-M. Kiessling, W. Miller, U. Rehse, O. Klein, Ch. Lechner, J. Sprekels, B. Nacke, H. Kasjanov, P. Lange, M. Ziem, B. Lux, M. Czupalla, O. Root, V. Trautmann, G. Bethin, *Crystal growth in heater-magnet modules — From concept to use*, in: Proceedings of the International Scientific Colloquium Modelling for Electromagnetic Processing (MEP2008), Hannover, October 26–29, 2008, E. Braake, B. Nacke, eds., Leibniz University of Hannover, 2008, pp. 79–84.

[13] P. Krejčí, *Hysteresis rarefaction in the Riemann problem*, in: International Workshop on Multi-Rate Processes and Hysteresis, March 31 – April 5, 2008, Cork, Ireland, vol. 138 of J. Phys.: Conf. Ser., Inst. Phys., 2008, pp. 012010/1–012010/10.

[14] C. Krüger, A. Demircan, G. Stibenz, N. Zhavoronkov, G. Steinmeyer, *Asymptotic pulse shapes in filamentary propagation of femtosecond pulses and self-compression*, in: Conference on Lasers and Electro-Optics/Quantum Electronics and Laser Science Conference, May 04–09, 2008, San Jose, CA, vol. 1–9 of IEEE Lasers and Electro-Optics Society (LEOS) Annual Meeting, IEEE, New York, NY, USA, 2008, pp. 2501–2502.

[15] M. Lichtner, M. Radziunas, U. Bandelow, M. Spreemann, H. Wenzel, *Dynamic simulation of high brightness semiconductor lasers*, in: Proceedings of the 8th International Conference on Numerical Simulation of Optoelectronic Devices, NUSOD'08, J. Piprek, E. Larkins, eds., IEEE/LEOS, 2008, pp. 65–66.

[16] Ch. Meyer, D. Hömberg, J. Rehberg, W. Ring, *Optimal control of the thermistor problem*, in: Optimal Control of Coupled Systems of PDE, Workshop, March 2–8, 2008, vol. 5 of Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach, 2008, pp. 624–626.

[17] A. Mielke, *Numerical approximation techniques for rate-independent inelasticity*, in: Proceedings of the IUTAM Symposium on Theoretical, Computational and Modelling Aspects of Inelastic Media, B.D. Reddy, ed., vol. 11 of IUTAM Bookseries, Springer, 2008, pp. 53–63.

[18] H.-J. Mucha, H.-G. Bartel, J. Dolata, *Effects of data transformation on cluster analysis of archaeometric data*, in: Data Analysis, Machine Learning and Applications, Ch. Preisnach, H. Burkhardt, L. Schmidt-Thieme, R. Decker, eds., Springer, Berlin, 2008, pp. 681–688.

[19] J. Behrndt, M. Malamud, H. Neidhardt, *Trace formula for dissipative and coupled scattering systems*, in: Spectral Theory in Inner Product Spaces and Applications, J. Behrndt, K.-H. Förster, H. Langer, C. Trunk, eds., vol. 188 of Operator Theory: Advances and Applications, Birkhäuser, Basel, 2008, pp. 57–93.

[20] P. Philip, *Optimal control of conduction-radiative temperature fields generated via electromagnetic heating*, in: Optimal Control of Coupled Systems of PDE, Workshop, March 2–8, 2008, vol. 5 of Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach, 2008, pp. 631–632.

[21] M. Pietrzyk, I. Kanattšikow, A. Demircan, *On the compression of ultrashort optical pulses beyond the slowly varying envelope approximation*, in: Proceedings of the 8th International Conference on Numerical Simulation of Optoelectronic Devices NUSOD'08, J. Piprek, E. Larkins, eds., IEEE/LEOS, 2008, pp. 59–60.

[22] J. Polzehl, V. Spokoiny, *Structural adaptive smoothing by propagation-separation methods*, in: Handbook of Data Visualization, Ch.-h. Chen, W. Härdle, A. Unwin, eds., Springer Handbooks of Computational Statistics, Springer, Berlin, Heidelberg, 2008, pp. 471–492.

[23] J. Franke, R. Dahlhaus, J. Polzehl, V. Spokoiny, G. Steidl, J. Weickert, A. Berdychevski, S. Didas, S. Halim, P. Mrázek, S.S. Rao, J. Tadjuidje, *Structural adaptive smoothing procedures*, in: Mathematical Methods in Time Series Analysis and Digital Image Processing, R. Dahlhaus, J. Kurths, P. Maass, J. Timmer, eds., Understanding Complex Systems, Springer, Berlin, Heidelberg, 2008, pp. 183–229.

[24] M. Radziunas, *Travelling wave modeling of semiconductor ring lasers*, in: Semiconductor Lasers and Laser Dynamics III, K.P. Panajotov, M. Sciamanna, A.A. Valle, R. Michalzik, eds., vol. 6997 of Proceedings of SPIE, SPIE, 2008, pp. 69971B/1–69971B/9.

[25] R. Model, A. Rathsfeld, H. Gross, M. Wurm, B. Bodermann, *A scatterometry inverse problem in optical mask metrology*, in: 6th International Conference on Inverse Problems in Engineering: Theory and Practice, 15–19 June 2008, Dourdan (Paris), France, vol. 135 of J. Phys.: Conf. Ser., Inst. Phys., 2008, pp. 012071/1–012071/8.

[26] O. Rott, P. Rasper, D. Hömberg, E. Uhlmann, *A milling model with thermal effects including the dynamics of machine and work piece*, Proceedings, 1st International Conference on Process Machine Interactions, Hannover, September 3–4, 2008, PZH Produktionstechnisches Zentrum GmbH, Garbsen, 2008, pp. 369–378.

[27] H. Si, J. Fuhrmann, K. Gärtner, *Boundary conforming Delaunay mesh generation*, in: Proceedings of the International Conference "Numerical Geometry, Grid Generation and High Performance Computing", Moscow, 10–13 June 2008, V.A. Garanzha, Y.G. Evtushenko, B.K. Soni, N.P. Weatherill, eds., 2008, pp. 230–237.

[28] A. Steinbrecher, *GEOMS: A new software package for the numerical simulation of multibody systems*, in: Proceedings, UKSim Tenth International Conference on Computer Modelling and Simulation, EUROSIM/UKSim 2008, Cambridge, UK, April 1–3, 2008, D. Al-Dabass, A. Orsoni, A. Brentnall, A. Abraham, R. Zobel, eds., IEEE, Piscataway, 2008, pp. 643–648.

Contributions to Collected Editions (to appear)

[1] H. Heitsch, R. Henrion, Ch. Küchler, W. Römisch, *Generierung von Szenariobäumen und Szenarioreduktion für stochastische Optimierungsprobleme in der Energiewirtschaft*, in: Dezentrale regenerative Energieversorgung: Innovative Modellierung und Optimierung, R. Schultz, H.-J. Wagner, eds., LIT Verlag, Münster.

[2] E. Holzbecher, *Numerical solutions for the Lévêque problem of boundary layer mass or heat flux and comparison with experiments*, in: European COMSOL Conference 2008, Hannover, COMSOL.

[3] A. Bradji, E. Holzbecher, *On the convergence order in Sobolev norms of COMSOL solutions*, in: COMSOL Conference 2008, Budapest, COMSOL.

[4] E. Holzbecher, H. Si, *Accuracy tests for COMSOL — and Delaunay meshes*, in: European COMSOL Conference 2008, Hannover, COMSOL.

[5] C. Krüger, A. Demircan, S. Skupin, G. Stibenz, N. Zhavoronkov, G. Steinmeyer, *Asymptotic pulse shapes and pulse self-compression in femtosecond filaments*, in: Ultrafast Phenomena XVI, Proceedings of the 16th International Conference.

[6] M. Lichtner, M. Spreemann, *Parallel simulation of high power semiconductor lasers*, in: Proceedings of PARA 2008, Lecture Notes in Computer Science, Springer, Berlin, Heidelberg.

[7] A. Mielke, *Lie groups in plasticity at finite strains*, in: Applied Dynamics and Geometric Mechanics, Workshop, July 21–25, 2008, Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach.

[8] H.-J. Mucha, H.-G. Bartel, J. Dolata, *Finding Roman brickyards in Germania Superior by model-based cluster analysis of archaeometric data*, in: Proceedings of Computer Applications and Quantitative Methods in Archaeology (CAA 2007).

[9] J. Dolata, H.-G. Bartel, H.-J. Mucha, *Geochemische und statistische Erkundung der Herstellungsorte von Ziegeln der legio XXI Rapax*, in: Monographie 74, Verlag des Römisch-Germanischen Zentralmuseums, Mainz.

[10] H. Gross, A. Rathsfeld, M. Bär, *Modelling and uncertainty estimates for numerically reconstructed profiles in scatterometry*, in: Proceedings of the Conference on Advanced Mathematical and Computational Tools in Metrology and Testing, Paris, June 23–25, 2008.

[11] B. Denkena, G. Günther, V. Mehrmann, H.-C. Möhring, A. Steinbrecher, *Kalibrierverfahren für hybride Parallelkinematiken*, in: Fertigungsmaschinen mit Parallelkinematiken — Forschung in Deutschland, U. Heisel, H. Weule, eds., Shaker-Verlag.

A.7 Preprints, Reports

A.7.1 WIAS Preprints Series[3]

[1] V.F. Butuzov, N.N. Nefedov, L. Recke, K.R. Schneider, *Existence and stability of solutions with periodically moving weak internal layers*, Preprint no. 1294, WIAS, Berlin, 2008.

[2] K. Fleischmann, L. Mytnik, V. Wachtel, *Hölder index for density states of (alpha,1,beta)-superprocesses at a given point*, Preprint no. 1385, WIAS, Berlin, 2008.

[3] ———, *Optimal Hölder index for density states of superprocesses with $(1+\beta)$-branching mechanism*, Preprint no. 1327, WIAS, Berlin, 2008.

[4] N.N. Nefedov, L. Recke, K.R. Schneider, *Exponential asymptotic stability via Krein–Rutman theorem for singularly perturbed parabolic periodic Dirichlet problems*, Preprint no. 1333, WIAS, Berlin, 2008.

[5] S. Amiranashvili, A.G. Vladimirov, U. Bandelow, *A model equation for ultrashort optical pulses*, Preprint no. 1348, WIAS, Berlin, 2008.

[6] L.-P. Arguin, *Competing particle systems and the Ghirlanda–Guerra identities*, Preprint no. 1303, WIAS, Berlin, 2008.

[7] D. Belomestny, J. Kampen, J.G.M. Schoenmakers, *Holomorphic transforms with application to affine processes*, Preprint no. 1297, WIAS, Berlin, 2008.

[8] D. Belomestny, A. Kolodko, J.G.M. Schoenmakers, *Pricing CMS spreads in the Libor market model*, Preprint no. 1386, WIAS, Berlin, 2008.

[9] A. Bianchi, A. Bovier, D. Ioffe, *Sharp asymptotics for metastability in the random field Curie–Weiss model*, Preprint no. 1342, WIAS, Berlin, 2008.

[10] M. Baake, M. Birkner, R.V. Moody, *Diffraction of stochastic point sets: Exactly solvable examples*, Preprint no. 1307, WIAS, Berlin, 2008.

[11] M. Birkner, J. Blath, M. Möhle, M. Steinrücken, J. Tams, *A modified lookdown construction for the Xi–Fleming–Viot process with mutation and populations with recurrent bottlenecks*, Preprint no. 1352, WIAS, Berlin, 2008.

[12] M. Birkner, A. Greven, F. den Hollander, *Quenched LDP for words in a letter sequence*, Preprint no. 1349, WIAS, Berlin, 2008.

[13] M. Birkner, R. Sun, *Annealed vs quenched critical points for a random walk pinning model*, Preprint no. 1350, WIAS, Berlin, 2008.

[14] A. Bovier, F. den Hollander, C. Spitoni, *Homogeneous nucleation for Glauber and Kawasaki dynamics in large volumes at low temperatures*, Preprint no. 1331, WIAS, Berlin, 2008.

[15] C. Brée, A. Demircan, S. Skupin, L. Bergé, G. Steinmeyer, *Self-pinching of pulsed laser beams in a plasma filament*, Preprint no. 1377, WIAS, Berlin, 2008.

[16] C. Brée, A. Demircan, G. Steinmeyer, *Method for computing the nonlinear refractive index via Keldysh theory*, Preprint no. 1388, WIAS, Berlin, 2008.

[17] W. Dreyer, F. Duderstadt, S.-J. Kimmerle, *A study on the eigenstrain problem in solid mixtures*, Preprint no. 1311, WIAS, Berlin, 2008.

[18] W. Dreyer, F. Duderstadt, S. Eichler, M. Naldzhieva, *On unwanted nucleation phenomena at the wall of a VGF chamber*, Preprint no. 1312, WIAS, Berlin, 2008.

[3] Preprints written by guests during their stay at WIAS have been listed in front of those written by the collaborators of WIAS.

[19] W. Dreyer, D. Hömberg, Th. Petzold, *A model for the austenite-ferrite phase transition in steel including misfit stress*, Preprint no. 1310, WIAS, Berlin, 2008.

[20] P.-E. Druet, *On weak solutions to the stationary MHD-equations coupled to heat transfer with nonlocal radiation boundary conditions*, Preprint no. 1290, WIAS, Berlin, 2008.

[21] M. Ehrhardt, *Nonlinear models in option pricing — An introduction*, Preprint no. 1332, WIAS, Berlin, 2008.

[22] X. Antoine, A. Arnold, Ch. Besse, M. Ehrhardt, A. Schädle, *A review of transparent and artificial boundary conditions techniques for linear and nonlinear Schrödinger equations*, Preprint no. 1313, WIAS, Berlin, 2008.

[23] A. Arnold, M. Ehrhardt, M. Schulte, *Numerical simulation of quantum waveguides*, Preprint no. 1339, WIAS, Berlin, 2008.

[24] A. Arnold, M. Ehrhardt, M. Schulte, I. Sofronov, *Discrete transparent boundary conditions for the Schrödinger equation on circular domains*, Preprint no. 1344, WIAS, Berlin, 2008.

[25] O. Gloger, M. Ehrhardt, Th. Dietrich, O. Hellwich, K. Graf, E. Nagel, *A threestepped coordinated level set segmentation method for identifying atherosclerotic plaques on MR-images*, Preprint no. 1317, WIAS, Berlin, 2008.

[26] M. Ehrhardt, H. Han, Ch. Zheng, *Numerical simulation of waves in periodic structures*, Preprint no. 1323, WIAS, Berlin, 2008.

[27] M. Ehrhardt, R. Mickens, *Fast, stable and accurate numerical method for the Black–Scholes equation of American options*, Preprint no. 1305, WIAS, Berlin, 2008.

[28] M. Ehrhardt, J. Sun, Ch. Zheng, *Evaluation of exact boundary mappings for one-dimensional semi-infinite periodic arrays*, Preprint no. 1358, WIAS, Berlin, 2008.

[29] M. Ehrhardt, Ch. Zheng, *Exact artificial boundary conditions for problems with periodic structures*, Preprint no. 1309, WIAS, Berlin, 2008.

[30] J. Ankudinova, M. Ehrhardt, *Fixed domain transformations and split-step finite difference schemes for nonlinear Black–Scholes equations for American options*, Preprint no. 1328, WIAS, Berlin, 2008.

[31] M. Ehrhardt, J. Fuhrmann, A. Linke, E. Holzbecher, *Mathematical modeling of channel-porous layer interfaces in PEM fuel cells*, Preprint no. 1375, WIAS, Berlin, 2008.

[32] M. Elagin, *Locally adaptive estimation methods with application to univariate time series*, Preprint no. 1383, WIAS, Berlin, 2008.

[33] M. Elagin, V. Spokoiny, *Locally time homogeneous time series modelling*, Preprint no. 1379, WIAS, Berlin, 2008.

[34] J. Elschner, M. Yamamoto, *Uniqueness in determining polyhedral sound-hard obstacles with a single incoming wave*, Preprint no. 1289, WIAS, Berlin, 2008.

[35] J. Elschner, G.C. Hsiao, A. Rathsfeld, *An optimisation method in inverse acoustic scattering by an elastic obstacle*, Preprint no. 1365, WIAS, Berlin, 2008.

[36] P. Ferrari, *Slow decorrelations in KPZ growth*, Preprint no. 1346, WIAS, Berlin, 2008.

[37] F. Bornemann, P. Ferrari, M. Prähofer, *The Airy$_1$ process is not the limit of the largest eigenvalue in GOE matrix diffusion*, Preprint no. 1345, WIAS, Berlin, 2008.

[38] A. Borodin, P. Ferrari, *Anisotropic growth of random surfaces in $2+1$ dimensions*, Preprint no. 1318, WIAS, Berlin, 2008.

[39] J. Fuhrmann, H. Zhao, E. Holzbecher, H. Langmach, M. Chojak, R. Halseid, Z. Jusys, R.J. Behm, *Experimental and numerical model study of the limiting current in a channel flow cell with a circular electrode*, Preprint no. 1301, WIAS, Berlin, 2008.

[40] A. Glitzky, *Analysis of a spin-polarized drift-diffusion model*, Preprint no. 1300, WIAS, Berlin, 2008.

[41] ———, *Exponential decay of the free energy for discretized electro-reaction-diffusion systems*, Preprint no. 1291, WIAS, Berlin, 2008.

[42] A. Glitzky, K. Gärtner, *Existence of bounded steady state solutions to spin-polarized drift-diffusion systems*, Preprint no. 1357, WIAS, Berlin, 2008.

[43] R. Henrion, J. Outrata, Th. Surowiec, *On the co-derivative of normal cone mappings to inequality systems*, Preprint no. 1321, WIAS, Berlin, 2008.

[44] R. Henrion, A. Seeger, *Uniform boundedness of norms of convex and nonconvex processes*, Preprint no. 1308, WIAS, Berlin, 2008.

[45] K. Hoke, H.-Chr. Kaiser, J. Rehberg, *Analyticity for some operator functions from statistical quantum mechanics*, Preprint no. 1373, WIAS, Berlin, 2008.

[46] H. Cornean, K. Hoke, H. Neidhardt, P.N. Racec, J. Rehberg, *A Kohn–Sham system at zero temperature*, Preprint no. 1293, WIAS, Berlin, 2008.

[47] A. Fasano, D. Hömberg, D. Naumov, *On a mathematical model for laser-induced thermotherapy*, Preprint no. 1368, WIAS, Berlin, 2008.

[48] D. Hömberg, Ch. Meyer, J. Rehberg, W. Ring, *Optimal control for the thermistor problem*, Preprint no. 1363, WIAS, Berlin, 2008.

[49] K. Chełminski, D. Hömberg, O. Rott, *On a thermomechanical milling model*, Preprint no. 1361, WIAS, Berlin, 2008.

[50] D. Hömberg, N. Togobytska, M. Yamamoto, *On the evaluation of dilatometer experiments*, Preprint no. 1298, WIAS, Berlin, 2008.

[51] J. Kampen, *Global regularity and probabilistic schemes for free boundary surfaces of multivariate American derivatives and their Greeks*, Preprint no. 1325, WIAS, Berlin, 2008.

[52] ———, *How to compute the length of a geodesic on a Riemannian manifold with small error in arbitrary Sobolev norms*, Preprint no. 1384, WIAS, Berlin, 2008.

[53] D. Knees, *Short note on global spatial regularity in elasto-plasticity with linear hardening*, Preprint no. 1337, WIAS, Berlin, 2008.

[54] D. Knees, Ch. Zanini, A. Mielke, *Crack growth in polyconvex materials*, Preprint no. 1351, WIAS, Berlin, 2008.

[55] Ch. Kraus, *Bernstein–Walsh type theorems for real analytic functions in several variables*, Preprint no. 1390, WIAS, Berlin, 2008.

[56] K. Hermsdörfer, Ch. Kraus, D. Kröner, *Interface conditions for limits of the Navier–Stokes–Korteweg model*, Preprint no. 1389, WIAS, Berlin, 2008.

[57] P. Krejčí, J.P. O'Kane, A. Pokrovskii, D. Rachinskii, *Stability results for a soil model with singular hysteretic hydrology*, Preprint no. 1341, WIAS, Berlin, 2008.

[58] P. Krejčí, L. Panizzi, *Regularity and uniqueness in quasilinear parabolic systems*, Preprint no. 1340, WIAS, Berlin, 2008.

[59] M. Eleuteri, J. Kopfová, P. Krejčí, *Magnetohydrodynamic flow with hysteresis*, Preprint no. 1319, WIAS, Berlin, 2008.

[60] C. Krüger, A. Demircan, G. Steinmeyer, *Asymptotic pulse shapes in filamentary propagation of intense femtosecond pulses*, Preprint no. 1359, WIAS, Berlin, 2008.

[61] M. Lichtner, M. Spreemann, *Parallel simulation of high power semiconductor lasers*, Preprint no. 1326, WIAS, Berlin, 2008.

[62] J.C. de los Reyes, Ch. Meyer, B. Vexler, *Finite element error analysis for state-constrained optimal control of the Stokes equations*, Preprint no. 1292, WIAS, Berlin, 2008.

[63] R. Griesse, Ch. Meyer, *Optimal control of static plasticity with linear kinematic hardening*, Preprint no. 1370, WIAS, Berlin, 2008.

[64] R. Haller-Dintelmann, Ch. Meyer, J. Rehberg, *Hölder continuity for second order elliptic problems with nonsmooth data*, Preprint no. 1316, WIAS, Berlin, 2008.

[65] A. Mielke, R. Rossi, G. Savaré, *Modeling solutions with jumps for rate-independent systems on metric spaces*, Preprint no. 1347, WIAS, Berlin, 2008.

[66] A. Mielke, U. Stefanelli, *A discrete variational principle for rate-independent evolution*, Preprint no. 1295, WIAS, Berlin, 2008.

[67] J. Giannoulis, M. Herrmann, A. Mielke, *Lagrangian and Hamiltonian two-scale reduction*, Preprint no. 1302, WIAS, Berlin, 2008.

[68] A. Mainik, A. Mielke, *Global existence for rate-independent gradient plasticity at finite strain*, Preprint no. 1299, WIAS, Berlin, 2008.

[69] A. Mielke, A. Petrov, J.A.C. Martins, *Convergence of solutions of kinetic variational inequalities in the rate-independent quasi-static limit*, Preprint no. 1322, WIAS, Berlin, 2008.

[70] A. Mielke, L. Paoli, A. Petrov, *On existence and approximation for a 3D model of thermally-induced phase transformations in shape-memory alloys*, Preprint no. 1330, WIAS, Berlin, 2008.

[71] J. Polzehl, K. Tabelow, *Structural adaptive smoothing in diffusion tensor imaging: The R package dti*, Preprint no. 1382, WIAS, Berlin, 2008.

[72] P.N. Racec, R. Racec, H. Neidhardt, *Evanescent channels and scattering in cylindrical nanowire heterostructures*, Preprint no. 1376, WIAS, Berlin, 2008.

[73] M. Radziunas, *Traveling wave modeling of dynamics in semiconductor ring lasers*, Preprint no. 1315, WIAS, Berlin, 2008.

[74] M. Radziunas, V.Z. Tronciu, U. Bandelow, M. Lichtner, M. Spreemann, H. Wenzel, *Mode transitions in distributed-feedback tapered master-oscillator power-amplifier*, Preprint no. 1366, WIAS, Berlin, 2008.

[75] R. Haller-Dintelmann, J. Rehberg, *Maximal parabolic regularity for divergence operators including mixed boundary conditions*, Preprint no. 1288, WIAS, Berlin, 2008.

[76] A. Rohde, *Adaptive goodness-of-fit tests based on signed ranks*, Preprint no. 1355, WIAS, Berlin, 2008.

[77] ———, *Sharp-optimal adjustment for multiple testing in the multivariate two-sample problem*, Preprint no. 1356, WIAS, Berlin, 2008.

[78] A. Rohde, L. Dümbgen, *Confidence sets for the optimal approximating model — Bridging a gap between adaptive point estimation and confidence regions*, Preprint no. 1354, WIAS, Berlin, 2008.

[79] O. Rott, P. Rasper, D. Hömberg, E. Uhlmann, *A milling model with thermal effects including the dynamics of machine and work piece*, Preprint no. 1338, WIAS, Berlin, 2008.

[80] K. Sabelfeld, *A stochastic fractal model of the universe related to the fractional Laplacian*, Preprint no. 1364, WIAS, Berlin, 2008.

[81] ———, *Stokes flows under random boundary velocity excitations*, Preprint no. 1362, WIAS, Berlin, 2008.

[82] K. Sabelfeld, O. Kurbanmuradov, A. Levykin, *Stochastic simulation of flows and particle transport in porous tubes*, Preprint no. 1324, WIAS, Berlin, 2008.

[83] O. Kurbanmuradov, K. Sabelfeld, *Stochastic flow simulation and particle transport in a 2D layer of random porous medium*, Preprint no. 1374, WIAS, Berlin, 2008.

[84] I. Shalimova, K. Sabelfeld, *Elastic half-plane under random boundary excitations*, Preprint no. 1314, WIAS, Berlin, 2008.

[85] ———, *Elastostatics of a half-plane under random boundary excitations*, Preprint no. 1343, WIAS, Berlin, 2008.

[86] ———, *Stochastic analysis of an elastic 3D half-space respond to random boundary displacements: Exact results and Karhunen–Loéve expansion*, Preprint no. 1387, WIAS, Berlin, 2008.

[87] F. Schmid, *Quasi-static contact problem with finitely many degrees of freedom and dry friction*, Preprint no. 1336, WIAS, Berlin, 2008.

[88] G. Schmidt, *Integral equations for conical diffraction by coated gratings*, Preprint no. 1296, WIAS, Berlin, 2008.

[89] M. Herrmann, A. Segatti, *Infinite harmonic chain with heavy mass*, Preprint no. 1367, WIAS, Berlin, 2008.

[90] N. Serdyukova, *Dependence on the dimension for complexity of approximation of random fields*, Preprint no. 1360, WIAS, Berlin, 2008.

[91] H. Si, *Constrained Delaunay tetrahedral mesh generation and refinement*, Preprint no. 1372, WIAS, Berlin, 2008.

[92] ———, *The existence of triangulations of non-convex polyhedra without new vertices*, Preprint no. 1329, WIAS, Berlin, 2008.

[93] J. Sprekels, H. Wu, *A note on a parabolic equation with nonlinear dynamical boundary condition*, Preprint no. 1378, WIAS, Berlin, 2008.

[94] O. Anoschenko, E. Khruslov, H. Stephan, *Global weak solutions of the Navier–Stokes–Vlasov–Poisson system*, Preprint no. 1335, WIAS, Berlin, 2008.

[95] K. Tabelow, V. Piëch, J. Polzehl, H.U. Voss, *High resolution fMRI: Overcoming the signal-to-noise problem*, Preprint no. 1353, WIAS, Berlin, 2008.

[96] P. Suwanpinij, N. Togobytska, Ch. Keul, W. Weiss, U. Prahl, D. Hömberg, W. Bleck, *Phase transformation modeling and parameter identification from dilatometric investigations*, Preprint no. 1306, WIAS, Berlin, 2008.

[97] A.G. Vladimirov, A. Pimenov, D. Rachinskii, *Bifurcations in a model of monolithic passively mode-locked semiconductor laser*, Preprint no. 1334, WIAS, Berlin, 2008.

[98] G. Kitavtsev, B. Wagner, *Coarsening dynamics of slipping droplets*, Preprint no. 1381, WIAS, Berlin, 2008.

[99] M. Rauscher, R. Blossey, A. Münch, B. Wagner, *Spinodal dewetting of thin films with large interfacial slip: Implications from the dispersion relation*, Preprint no. 1380, WIAS, Berlin, 2008.

[100] W. Wagner, *Deviational particle Monte Carlo for the Boltzmann equation*, Preprint no. 1320, WIAS, Berlin, 2008.

[101] O. Muscato, V. Di Stefano, W. Wagner, *Numerical study of the systematic error in Monte Carlo schemes for semiconductors*, Preprint no. 1371, WIAS, Berlin, 2008.

[102] A. Weiss, *Escaping the Brownian stalkers*, Preprint no. 1304, WIAS, Berlin, 2008.

[103] X. Yao, J. Chen, Ch. Zhang, Y. Li, *On the clustering property of the random intersection graphs*, Preprint no. 1369, WIAS, Berlin, 2008.

A.7.2 WIAS Technical Reports Series

[1] D. Hoffmann, K. Tabelow, *Structural adaptive smoothing for single-subject analysis in SPM: The aws4SPM-toolbox*, WIAS Report no. 11, WIAS, Berlin, 2008.

A.7.3 Preprints/Reports in other Institutions

[1] S. Amiranashvili, U. Bandelow, A.G. Vladimirov, *Solitary wave solutions for few-cycle optical pulses*, Preprint no. 500, DFG Research Center Matheon, Berlin, 2008.

[2] P.-E. Druet, J. Naumann, J. Wolf, *A Meyers' type estimate for weak solutions to a generalized stationary Navier–Stokes system*, Preprint no. 06, Humboldt-Universität zu Berlin, Institut für Mathematik, 2008.

[3] X. Blanc, C. Le Bris, F. Legoll, C. Patz, *Finite-temperature coarse-graining of one-dimensional models: Mathematical analysis and computational approaches*, RR–6544, INRIA — Institut National de Recherche en Informatique et en Automatique, Le Chesnay, France, 2008.

[4] N. Suciu, C. Vamos, H. Vereecken, K. Sabelfeld, P. Knabner, *Dependence on initial conditions, memory effects, and ergodicity of transport in heterogeneous media*, Preprint no. 324, Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Angewandte Mathematik, 2008.

[5] F. Lanzara, V. Maz'ya, G. Schmidt, *Approximate Hermite quasi-interpolation (electronic only)*, arXiv:0806.2546, Cornell University Library, arXiv.org, UK, 2008.

[6] P. Cizek, W. Härdle, V. Spokoiny, *Adaptive pointwise estimation in time-inhomogeneous time-series models*, Discussion Paper no. 2008-002, Humboldt-Universität zu Berlin, SFB 649, 2008.

[7] B. Denkena, G. Günther, V. Mehrmann, H.-C. Möhring, A. Steinbrecher, *Kalibrierverfahren für hybride Parallelkinematiken*, Technical Report no. 02, Technische Universität Berlin, Institut für Mathematik, 2008.

[8] M.S. Celnik, R.I. Patterson, M. Kraft, W. Wagner, *A predictor-corrector algorithm for the coupling of stiff ODEs to a particle population balance*, Preprint no. 58, Cambridge Center for Computational Chemical Engineering, UK, 2008.

A.8 Talks, Posters, and Contributions to Exhibitions

A.8.1 Scientific Talks (Invited)[4]

1. O. Zindy, *Aging for random walks in random environment in the sub-ballistic regime*, Université Henri Poincaré, Nancy, France, January 31.
2. ———, *Aging for random walks in random environment in the sub-ballistic regime*, University of Cambridge, Faculty of Mathematics, UK, February 5.
3. O. Zindy, Ch. Sabot, *Random walk in random environment on Z in the sub-ballistic regime (scaling limit, renewal theory, aging phenomenon, quenched localization)*, 4 talks, Workshop "Marches Aléatoires, Milieux Aléatoires, Renforcement (Projet ANR: MEMEMO)", Université de Brest, Laboratoire de Mathématiques, France, May 26–30.
4. L.-P. Arguin, *On the ultrametricity of the Gibbs state in spin glasses*, Probability Seminar, Stanford University, Department of Mathematics, USA, February 11.
5. ———, *Competing particle systems*, Probability Seminar, New York University, Courant Institute of Mathematical Sciences, USA, February 15.
6. ———, *The structure of quasi-stationary competing particle systems*, Seminar "Stochastische Prozesse", Universität Zürich, Mathematisch-Naturwissenschaftliche Fakultät, Switzerland, March 5.
7. ———, *Ultrametricity from robust stochastic stability*, YEP (Young European Probabilists) – V Workshop "Statistical Mechanics on Random Structures" (YEP 2008), March 10–14, EURANDOM, Eindhoven, The Netherlands, March 13.
8. U. Bandelow, *Quantum-classical coupling in multi quantum well lasers*, 4th Workshop "Mathematical Models for Transport in Macroscopic and Mesoscopic Systems", February 7–10, WIAS, Berlin, February 8.
9. ———, *Modellierung und Simulation von Halbleiterlasern*, Graduate College of the Collaborative Research Center SFB 787 "Semiconductor Nanophotonics: Materials, Models, Devices", May 21–23, Technische Universität Berlin, Institut für Festkörperphysik, Graal-Müritz, May 23.
10. ———, *Short pulses in nonlinear optical fibers: Models and applications*, Colloquium "Nonlinear Dynamics in Complex Optical Systems", Humboldt-Universität zu Berlin, Institut für Physik, June 19.
11. ———, *Dynamic simulation of high brightness semiconductor lasers*, 8th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD) 2008, September 1–5, University of Nottingham, UK, September 2.
12. ———, *Modeling and analysis of master-oscillator power-amplifier seminconductor lasers*, University of Washington, Seattle, USA, October 16.
13. D. Belomestny, *Analytic transforms with application to affine Feller processes in finance*, 8th German Open Conference on Probability and Statistics, March 6–7, Rheinisch-Westfälische Technische Hochschule Aachen, March 6.
14. ———, *New series representations for the characteristic functions of affine Feller processes with applications to option pricing*, Financial and Actuarial Mathematics, September 22–26, Technical University of Vienna, Austria, September 23.
15. ———, *True upper bounds for Bermudan products via non-nested Monte Carlo*, West LB, Düsseldorf, November 17.

[4] Talks given by Weierstrass Fellowship holders during their stay at WIAS have been listed in front of those given by the collaborators of WIAS.

16. A. Bianchi, *Sharp asymptotics for metastability in the random field Curie–Weiss model*, Workshop on Metastability, January 9–11, EURANDOM, Eindhoven, The Netherlands, January 9.

17. ———, *Metastable exit times in the random field Curie–Weiss model*, Workshop GREFI-MEFI 2008: From Dynamical Systems to Statistical Mechanics, February 4 – March 7, Centre International de Rencontres Mathèmatiques (CIRM), Marseille, France, March 6.

18. ———, *Metastable exit times in the random field Curie–Weiss model*, YEP (Young European Probabilists) – V Workshop "Statistical Mechanics on Random Structures" (YEP 2008), March 10–14, EURANDOM, Eindhoven, The Netherlands, March 10.

19. ———, *Metastable exit times in the random field Curie–Weiss model*, Workshop on Random Systems from Physics to Biology, March 17–20, Technische Universität Berlin, Institut für Mathematik, March 19.

20. ———, *Metastability in the random field Curie–Weiss model*, Technion Probability and Stochastic Processes Seminar, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, May 20.

21. ———, *Coupling in potential wells: From average to pointwise estimates of metastable times*, Workshop on Random Dynamical Systems, November 17–19, Universität Bielefeld, Fakulät für Mathematik, November 17.

22. ———, *Coupling in potential wells: From average to pointwise estimates of metastable times*, Oberseminar Stochastik, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Angewandte Mathematik, November 20.

23. M. Birkner, *Computing likelihoods under Lambda-coalescents*, Statistisches Kolloquium, Heinrich-Heine Universität Düsseldorf, Mathematisch-Naturwissenschaftliche Fakultät, January 21.

24. ———, *Conditional LDP for sentences and directed polymers in random environment*, 8th German Open Conference on Probability and Statistics, March 4–7, Rheinisch-Westfälische Technische Hochschule Aachen, March 6.

25. ———, *Conditional LDP for sentences and directed polymers in random environment*, Workshop on Random Systems from Physics to Biology, March 17–20, Technische Universität Berlin, Institut für Mathematik, March 18.

26. ———, *Inference for Lambda-coalescents*, ESI Workshop "Frontiers in Mathematical Biology", April 14–19, Erwin Schrödinger International Institute for Mathematical Physics (ESI), Austria, April 16.

27. ———, *Lambda-coalescents and population genetics*, Ecole d'été de l'ANR MAEV "Biologie de l'Evolution et Modèles Probabilistes", September 15–19, La Londe Les Maures, France, September 15.

28. ———, *Diffraction of stochastic point sets: Exactly solvable examples*, Workshop on Symmetries and Invariants of Dynamical Systems, September 24–26, Universität Bielefeld, Institut für Mathematik, September 26.

29. ———, *Inference for Lambda-coalescents*, Workshop on Population Genetics: Statistical Methods and Applications in Human Disease, Immunology and Evolution, November 12–14, University of Aarhus, Thiele Center for Applied Mathematics in Natural Science, Denmark, November 13.

30. ———, *Locally regulated populations and ancestral lineages*, Seminar on Stochastic Processes, Eidgenössische Technische Hochschule Zürich, Switzerland, December 3.

31. ———, *Conditional LDP for sentences and applications to disordered spatial systems*, Workshop "Statistical Mechanics" of the Semester "Interacting Particle Systems, Statistical Mechanics and Probability Theory", December 8–12, Institut Henri Poincaré, Centre Émile Borel, Paris, France, December 9.

32. A. Bovier, *Universality of REM-like ageing in mean field spin glasses*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät I, January 15.

33. ———, *Universality of Lévy processes in ageing systems*, YEP (Young European Probabilists) – V Workshop "Statistical Mechanics on Random Structures" (YEP 2008), March 10–14, EURANDOM, Eindhoven, The Netherlands, March 14.

34. ———, *Universality of Lévy processes in mean field spin glasses*, Workshop "Stochastic Analysis", June 1–7, Mathematisches Forschungsinstitut Oberwolfach, June 6.

35. ———, *Introduction to the Statistical Mechanics of Spin Glasses*, 3 talks, Summer School in Mathematical Physics, Workshop "Rigorous Results in Statistical Mechanics and Quantum Field Theory", Feza Gürsey Institute, Istanbul, Turkey, June 12–20.

36. ———, *Homogeneous nucleation in Kawasaki dynamics*, 7th World Congress in Probability and Statistics, July 14–19, National University of Singapore, Department of Statistics and Applied Probability, Department of Mathematics, and Institute for Mathematical Sciences, Singapore, July 16.

37. W. Dreyer, *On the entropy inequality. From its historical origins to modern applications*, Third Workshop "Micro-Macro Modelling and Simulation of Liquid-Vapour Flows", January 24–25, Centre National de la Recherche Scientifique, Strasbourg, France, January 25.

38. ———, *From the global entropy inequality to kinetic relations*, Mini-workshop "Hyperbolic Aspects of Phase Transition Dynamics", February 24 – March 1, Mathematisches Forschungsinstitut Oberwolfach, February 28.

39. ———, *Thermodynamic needs versus capabilities of micro-macro transitions*, 2008 SIAM Conference on Mathematical Aspects of Materials Science, May 11–14, Philadelphia, USA, May 13.

40. ———, *The triple-point problem for crystal growth of gallium arsenide*, Freiberger Compound GmbH, June 12.

41. ———, *Phase field models and corresponding Gibbs–Thomson laws. Part I*, SIMTECH Seminar Multiscale Modelling in Fluid Mechanics, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, November 5.

42. ———, *Phase transitions and hysteresis inside the cathode of lithium ion batteries*, International Workshop on Fundamentals of Lithium-based Batteries, November 23–28, Tegernsee, November 25.

43. ———, *The storage of hydrogen in crystals*, 21. Workshop "Composite-Forschung in der Mechanik", December 1–3, Institut für Technische Mechanik, Universität Karlsruhe (TH), Bad Herrenalb, December 2.

44. P.-E. Druet, *On weak solutions to the system of magnetohydrodynamics coupled to heat transfer, including nonlocal radiation effects*, Oberseminar Analysis, Technische Universität Dresden, Institut für Analysis, January 31.

45. ———, *Weak solutions to a model for global heat transfer arising in crystal growth from the melt with applied magnetic fields*, Workshop "Optimal Control of Coupled Systems", March 2–7, Mathematisches Forschungsinstitut Oberwolfach, March 5.

46. F. Duderstadt, *On the growth of the water droplets in wet air*, Third Workshop "Micro-Macro Modelling and Simulation of Liquid-Vapour Flows", January 24–25, Centre National de la Recherche Scientifique, Strasbourg, France, January 23.

47. ———, *Keimbildung bei Fest-Flüssig-Phasenübergängen von Galliumarsenid*, 21. Workshop "Composite-Forschung in der Mechanik", December 1–3, Institut für Technische Mechanik, Universität Karlsruhe (TH), Bad Herrenalb, December 2.

48. M. Ehrhardt, *The numerical solution of nonlinear Black–Scholes equations*, 4th Workshop on Nonlinear PDEs and Financial Mathematics, April 3–4, Halmstad University, Sweden, April 3.

49. ———, *Numerische Lösung von PDGln auf unbeschränkten Gebieten und Level-Set-Methoden in der medizinischen Bildverarbeitung*, Universität Koblenz-Landau, April 9.

50. ———, *Numerical solution of periodic structure problems*, Comenius University, Bratislava, Slovakia, June 4.

51. ———, *Numerical simulation of periodic structure problems*, École Nationale Supérieure de Techniques Avancées (ENSTA), Paris, France, June 19.

52. ———, *Numerische Lösung von PDGln auf unbeschränkten Gebieten*, Carl von Ossietzky Universität Oldenburg, August 28.

53. ———, *Numerical simulation of coupled flow in porous media*, Université des Sciences et Technologies de Lille, Laboratoire Paul Painlevé, INRIA SIMPAF Team, France, September 24.

54. ———, *Numerische Lösung von PDGln auf unbeschränkten Gebieten mit Anwendungen in der Physik*, Heinrich-Heine-Universität Düsseldorf, October 1.

55. ———, *On the numerical solution of nonlinear Black–Scholes equations*, Johann Wolfgang Goethe-Universität, Frankfurt am Main, October 6.

56. ———, *Numerische Lösung von PDGln auf unbeschränkten Gebieten*, Bergische Universität Wuppertal, October 24.

57. ———, *Numerical methods in finance (block lecture)*, 11 talks, Master's Program in Financial Mathematics, Halmstad University, Sweden, November 2–12.

58. ———, *Mathematical modeling of channel — Porous layer interfaces in PEM fuel cells*, Fundamentals and Developments of Fuel Cells 2008 Conference (FDFC2008), December 10–12, Nancy, France, December 12.

59. J. Ehrt, *Normally hyperbolic manifolds for viscous balance laws*, Work Seminar "Modelling, Analysis and Simulation", Centrum voor Wiskunde & Informatica, Amsterdam, The Netherlands, August 22.

60. ———, *Semi-strong interaction of pulses*, Work Seminar "Modelling, Analysis and Simulation", Centrum voor Wiskunde & Informatica, Amsterdam, The Netherlands, October 23.

61. J. Elschner, *Direct and inverse problems in fluid-solid interaction*, Workshop "Analysis of Boundary Element Methods", April 14–18, Mathematisches Forschungsinstitut Oberwolfach, April 18.

62. P. Ferrari, *Universality of the Airy processes along space-like paths*, Conference on Random Matrices: Probabilistic Aspects and Applications, January 14–18, Rheinische Friedrich-Wilhelms-Universität Bonn, January 15.

63. ———, *Large time asymptotics of growth models on space-like paths*, 8th German Open Conference on Probability and Statistics, March 4–7, Rheinisch-Westfälische Technische Hochschule Aachen, March 5.

64. ———, *Large time asymptotics of growth models on space-like paths*, Workshop on Random Systems from Physics to Biology, March 17–20, Technische Universität Berlin, Institut für Mathematik, March 19.

65. ———, *Large time asymptotics of growth models on space-like paths*, Probability 2008: New Scaling Limits and Other Recent Developments, March 31 – April 4, University of Warwick, Department of Statistics, UK, April 1.

66. ———, *Anisotropic growth of random surfaces in 2+1 dimensions*, Mathematical Physics Seminar, Technische Universität München, May 16.

67. ———, *Anisotropic growth of random surfaces in 2+1 dimensions*, Geometry, Physics and Probability Seminar, May 19–24, Université Catholique de Louvain, Belgium, May 22.

68. ———, *Random matrices and related problems*, 7 talks, 2008 Beg Rohu Summer School of Statistical Physics and Condensed Matter: Manifolds in Random Media, Random Matrices and Extreme Value Statistics, Ecole Nationale de Voile, Quiberon, France, June 16–28.

69. ———, *Anisotropic growth of random surfaces in 2+1 dimensions*, Workshop on Random Tilings, Random Partitions and Stochastic Growth Processes, September 1–6, Université de Montréal, Centre de Recherches Mathématiques, Canada, September 5.

70. J. Fuhrmann, *Numerical modeling of thin layer flow cells*, Universität Münster, Fachbereich Mathematik, January 23.

71. ———, *Numerical calculation of limiting current and kinetic parameters in thin layer flow cells*, 5th Symposium on Fuel Cell Modelling and Experimental Validation, March 11–12, Winterthur, Switzerland, March 12.

72. ———, *Electrochemistry, flow, and porous media: Aspects of numerical modeling*, Universität Stuttgart, Institut für Wasserbau, December 9.

73. K. Gärtner, *The van Roosbroeck system, some of its mathematical properties and their use in device simulation tools*, International Workshop on Semiconductor Pixel Detectors for Particles and Imaging (Pixel 2008), September 23–26, Fermi National Accelerator Laboratory, Batavia, Illinois, USA, September 26.

74. ———, *Existence of bounded discrete steady state solutions of the van Roosbroeck system on boundary conforming Delaunay grids*, Friedrich-Alexander-Universität Erlangen-Nürnberg, November 18.

75. E. Giacomini, *Dynamic semiparametric factor modus in risk preferences estimation*, 2008 North American Winter Meetings of the Econometric Society, January 4–6, North American Econometric Society, New Orleans, USA, January 6.

76. A. Glitzky, *Energy estimates for space and time discretized electro-reaction-diffusion systems*, Conference on Differential Equations and Applications to Mathematical Biology, June 23–27, Université Le Havre, France, June 26.

77. ———, *Energy estimates for continuous and discretized reaction-diffusion systems in heterostructures*, Annual Meeting of the Deutsche Mathematiker-Vereinigung 2008, minisymposium "Analysis of Reaction-Diffusion Systems with Internal Interfaces", September 15–19, Friedrich-Alexander-Universität Erlangen-Nürnberg, September 15.

78. J.A. Griepentrog, *Analysis and numerics for nonlocal phase separation processes in multicomponent systems*, Humboldt-Universität zu Berlin, February 14.

79. R. Henrion, *On calculating the normal cone to a finite union of convex polyhedra*, World Congress of Nonlinear Analysts (WCNA 2008), July 2–9, Orlando, USA, July 3.

80. ———, *On a dynamical model for chance constrained programming*, Conference on Optimization & Practices in Industry (COPI08), November 26–28, Clamart, France, November 28.

81. E. Holzbecher, *Multiphysics modeling*, Universität Stuttgart, May 30.

82. ———, *Groundwater flow and transport modelling using COMSOL/FEMLAB, Part V (block lecture)*, 15 talks, Polish Geological Institute, Pomeranian Branch, Szczecin, June 16–20.

83. ———, *Direct and inverse modeling of permeable porous media*, Institut für Isotopenforschung Leipzig, September 1.

84. D. Hömberg, *Solid-solid phase transitions — Analysis, optimal control and industrial application*, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, February 14.

85. ———, *Modellierung und Optimierung der Gefügeumwandlung in niedrig legierten Stählen und Anwendungen*, Salzgitter Mannesmann Forschung GmbH, February 19.

86. ———, *The heat treatment of steel — A mathematical control problem*, 2nd International Conference on Distortion Engineering 2008, September 17–19, Bremen, September 19.

87. ———, *On a mathematical model for high-speed milling including the dynamics of machine and workpiece*, Conference "Direct, Inverse and Control Problems for PDE's" (DICOP 08), September 22–26, Cortona, Italy, September 26.

88. ———, *Prozesskette Stahl*, Workshop of MATHEON with Siemens AG (Industry Sector) in cooperation with Center of Knowledge Interchange (CKI) of Technische Universität (TU) Berlin and Siemens AG, TU Berlin, September 29.

89. E. HÖSCHELE, *Fluid-structure interaction in forward roller coating*, industrial partner, Poing, May 13.

90. ———, *Einführung in die mathematische Modellierung und Simulation von Flüssig-Flow-Interaktion*, 3 talks, industrial partner, Poing, December 9–11.

91. H.-CHR. KAISER, *A drift-diffusion model for semiconductors with internal interfaces*, Annual Meeting of the Deutsche Mathematiker-Vereinigung 2008, Minisymposium "Analysis of Reaction-Diffusion Systems with Internal Interfaces", September 15–19, Friedrich-Alexander-Universität Erlangen-Nürnberg, September 15.

92. J. KAMPEN, *Higher order WKB expansions of the fundamental solution and pricing of options*, Credit Suisse, Zurich, Switzerland, March 28.

93. I. KANATTŠIKOW, *On the generalized Dirac bracket in the degenerate De Donder–Weyl Hamiltonian theory*, 40th Symposium on Mathematical Physics "Geometry & Quanta", June 25–28, Nicolaus Copernicus University, Toruń, Poland, June 28.

94. ———, *The short pulse equation: Integrability and generalizations*, Gdańsk University of Technology, Institute of Theoretical Physics and Quantum Informatics, Gdańsk, Poland, June 30.

95. ———, *Quantum gravity and emergent space-time from De Donder–Weyl quantization*, 4th International Workshop "From Quantum Mechanics through Complexity to Spacetime: The Role of Emergent Dynamical Structures" (DICE2008), September 22–26, University of Pisa, Castiglioncello, Italy, September 26.

96. O. KLEIN, *Outward pointing properties for vectorial hysteresis operators and some applications*, International Workshop on Multi-Rate Processes & Hysteresis, March 31 – April 5, University College Cork, Ireland, April 4.

97. D. KNEES, *Crack propagation in polyconvex materials*, Kolloquium Mechanik, Ruhr-Universität Bochum and Technische Universität Dortmund, Bochum, June 25.

98. ———, *On global spatial regularity in elasto-plasticity*, Seminar of the Collaborative Research Center (SFB) 611 "Singular Phenomena and Scaling in Mathematical Models", Universität Bonn, July 15.

99. ———, *On global spatial regularity in elasto-plasticity*, Seminar of Work Group PDE, November 4–5, Technische Universität Darmstadt, Fachbereich Mathematik, November 5.

100. TH. KOPRUCKI, *Band gap estimates for kp-Schrödinger operators*, May 19–23, Université de Rennes, Institut de Recherche Mathématique de Rennes, France, May 20.

101. M. KORZEC, *On sixth-order equations modeling the growth of self-assembled nano-structures*, Young Mathematicians Meet in Bonn, July 3–5, Universität Bonn, July 4.

102. ———, *Comparison of two Cahn–Hilliard type equations*, Summer Program "Geometrical Singularities and Singular Geometries", July 14–25, University of Minnesota, Institute for Mathematics and its Applications, Minneapolis, USA, July 21.

103. CH. KRAUS, *Ein Phasenfeldmodell vom Cahn-Hilliard-Typ im singulären Grenzwert*, Oberseminar Analysis, Universität Regensburg, Fakultät für Mathematik, April 25.

104. ———, *Phase field models and corresponding Gibbs–Thomson laws. Part II*, SIMTECH Seminar Multiscale Modelling in Fluid Mechanics, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, November 5.

105. P. Krejčí, *The Skorokhod problem and stability of discrete linear dynamical systems (in Czech)*, Seminar on Functional Analysis, Academy of Sciences of the Czech Republic, Mathematical Institute, Prague, January 8.

106. ———, *Lower dimensional nonequilibrium elastoplasticity*, Seminar on Analysis and Differential Equations, University of Lisbon, Centre of Mathematics and Applications, Portugal, January 23.

107. ———, *Evolution variational inequalities with state dependent constraints*, Seminar on Analysis, Geometry and Physico-Mathematics, University of Minho, Centre of Mathematics, Braga, Portugal, January 24.

108. ———, *Well-posedness of singular differential equations with hysteresis*, International Workshop on Multi-Rate Processes & Hysteresis, March 31 – April 5, University College Cork, Ireland, March 31.

109. ———, *Phase field systems with spatially nonlocal interaction*, Fudan University, School of Mathematical Sciences, Shanghai, China, May 13.

110. ———, *Temperature dependent hysteresis in thermoplasticity models, and their compatibility with thermodynamic principles*, Donghua University, Institute of Mathematics, Songjiang, China, May 16.

111. ———, *Kurzweil integral variational inequalities*, Hohai University, Institute of Mathematics, Nanjing, China, May 19.

112. ———, *Smooth and nonsmooth evolution quasivariational inequalities*, 9ème Colloque Franco-Roumain de Mathématiques Appliquées, August 28 – September 2, Brasov, Romania, September 1.

113. ———, *Uniqueness in nonlinearly coupled PDE systems*, Direct, Inverse and Control Problems for PDE's (DICOP 08), September 22–26, Cortona, Italy, September 26.

114. ———, *Oscillating lower dimensional elastoplastic structures*, Oberseminar Analysis, Technische Universität Dresden, Institut für Analysis, November 14.

115. ———, *Asymptotic behavior of processes in media with hysteresis*, Settima Giornata di Studio "Equazioni Differenziali e Calcolo delle Variazioni", Politecnico di Milano/Università di Pavia, Pavia, November 28.

116. C. Krüger, *Asymptotic pulse shapes in filamentary propagation of femtosecond pulses*, Max-Planck-Institut für Physik komplexer Systeme, Dresden, March 31.

117. M. Lichtner, *Modeling and parallel simulation of high power semiconductor lasers*, PARA 2008: Workshop on State-of-the-Art in Scientific and Parallel Computing, Minisymposium on Applications of Parallel Computation in Industry and Engineering, May 13–16, Trondheim, Norway, May 14.

118. A. Linke, *Mass conservative coupling of fluid flow and species transport in electrochemical flow cells*, Georg-August-Universität Göttingen, November 11.

119. P. Mathé, *On non-stability of some inverse problem in option pricing*, Workshop on Inverse and Partial Information Problems: Methodology and Applications, October 27–31, Austrian Academy of Sciences, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, October 30.

120. Ch. Meyer, *Optimal control of the thermistor problem*, Universität Bayreuth, Institut für Mathematik, February 7.

121. ———, *Optimal control of the thermistor problem*, Workshop "Optimal Control of Coupled Systems of PDE", March 2–8, Mathematisches Forschungsinstitut Oberwolfach, March 3.

122. ———, *Optimal control of the thermistor problem*, SIAM Conference on Optimization, May 10–13, Boston, USA, May 12.

123. ———, *Optimalsteuerung von PDEs mit Zustandsbeschränkungen — Anwendungen, Theorie, Numerik*, Rheinisch-Westfälische Technische Hochschule Aachen, Lehrstuhl für Numerische Mathematik, June 3.

124. ———, *Optimalsteuerung mit Zustandsbeschränkungen — Anwendungen, Theorie, Numerik*, Technische Universität Darmstadt, Fachbereich Mathematik, June 10.

125. ———, *Optimal control of the thermistor problem*, Universität der Bundeswehr München, Institut für Mathematik und Bauinformatik, July 9.

126. ———, *Finite element error analysis for state-constrained optimal control of the Stokes problem*, Annual Meeting of the Deutsche Mathematiker-Vereinigung 2008, Minisymposium "Optimal Control of PDEs with Pointwise State Constraints", September 15–19, Friedrich-Alexander-Universität Erlangen-Nürnberg, September 19.

127. A. Mielke, *Multiscale methods for Hamiltonian systems*, Collaborative Research Center (SFB) 647 "Space – Time – Matter: Analytic and Geometric Structures", Freie Universität Berlin, January 8.

128. ———, *Numerical approaches to rate-independent material models*, IUTAM Symposium on Theoretical, Modelling and Computational Aspects of Inelastic Media, January 13–18, University of Cape Town, CERECAM, South Africa, January 17.

129. ———, *Modeling for multifunctional materials: How to describe evolving microstructures in solids*, Workshop "Mathematics for Key Technologies and Innovation", February 21–22, Interdisciplinary Centre for Mathematical and Computational Modeling (ICM), University of Warsaw, Poland, February 21.

130. ———, *Multiscale methods for Hamiltonian systems*, University of Warsaw, Institute of Mathematics, Poland, February 22.

131. ———, *Classical rate-independent models including elastoplasticity*, Nečas Seminar on Continuum Mechanics, February 25 – March 16, Charles University Prague/Jindrich Nečas Center for Mathematical Modeling, Czech Republic, March 3.

132. ———, *The energetic formulation via functionals*, Nečas Seminar on Continuum Mechanics, February 25 – March 16, Charles University Prague/Jindrich Nečas Center for Mathematical Modeling, Czech Republic, March 4.

133. ———, *Applications in material models*, Nečas Seminar on Continuum Mechanics, February 25 – March 16, Charles University Prague/Jindrich Nečas Center for Mathematical Modeling, Czech Republic, March 10.

134. ———, *Gamma convergence for rate-independent processes and convergence of space-time discretization*, Nečas Seminar on Continuum Mechanics, February 25 – March 16, Charles University Prague/Jindrich Nečas Center for Mathematical Modeling, Czech Republic, March 11.

135. ———, *Wiggly energy landscapes and the origin of rate-independent friction*, 79th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2008), Session "Multiscales and Homogenization", March 31 – April 4, University of Bremen, April 2.

136. ———, *Multiscale modeling for shape-memory alloys: How to describe evolving microstructures in solids*, Graduate School Seminar, Rheinisch-Westfälische Technische Hochschule Aachen, Aachen Institute for Advanced Study in Computational Engineering Science, Center for Computational Engineering Science (AICES/CCES), April 21.

137. ———, *Multiscale methods for Hamiltonian systems and pulse interaction in periodic media*, Oberseminar für spezielle Probleme der Analysis, Rheinisch-Westfälische Technische Hochschule Aachen, Institut für Mathematik, April 22.

138. ———, *Global existence for rate-independent gradient plasticity at finite strain*, Oberseminar "Analysis", Technische Universität Dresden, Institut für Analysis, June 5.

139. ———, *Differential, energetic and metric formulations for rate-independent processes*, 6 talks, Summer Course on Nonlinear Partial Differential Equations and Applications, C.I.M.E. — Centro Internazionale Matematico Estivo, Cetraro (Cosenza), Italy, June 22–28.

140. ———, *Lie groups in plasticity at finite strains*, Workshop "Applied Dynamics and Geometric Mechanics", July 21–25, Mathematisches Forschungsinstitut Oberwolfach, July 21.

141. ———, *Hamiltonian passage from many-particle systems to PDEs*, 4 talks, BMS Summer School 2008: Mathematics of Multiscale Phenomena, Berlin Mathematical School/Freie Universität Berlin, Fachbereich Mathematik und Informatik, September 1–12.

142. ———, *Global energetic solutions for finite-strain plasticity with gradient regularization*, ISIMM Meeting STAMM XVI: Symposium on Trends in Applications of Mathematics to Mechanics, September 21–24, Università degli Studi di Trento, Centro Internazionale per la Ricerca Matematica, Levico Terme, Italy, September 22.

143. H.-J. Mucha, *Clustering a contingency table accompanied by visualization*, Annual Meeting of Gesellschaft für Klassifikation, July 16–18, Helmut-Schmidt-Universität, Hamburg, July 18.

144. M. Naldzhieva, *Analysis and applications of the Becker–Döring model*, Workshop "Mathematics for Key Technologies and Innovation", February 21–22, Interdisciplinary Centre for Mathematical and Computational Modeling (ICM), University of Warsaw, Poland, February 22.

145. H. Neidhardt, *On the trace formula for pairs of extensions*, Mathematical Physics and Spectral Theory, April 24–26, Humboldt-Universität zu Berlin, Workshop in Memory of Vladimir Geyler, April 26.

146. ———, *On the unitary equivalence of the absolutely continuous parts of self-adjoint extensions*, Annual Meeting of the Deutsche Mathematiker-Vereinigung 2008, Minisymposium "Operatortheorie", September 15–19, Friedrich-Alexander-Universität Erlangen-Nürnberg, September 19.

147. ———, *Scattering theory for open quantum systems*, Centre National de la Recherche Scientifique, Luminy, Centre de Physique Théorique, Marseille, France, October 22.

148. ———, *Kohn–Sham systems at zero temperature*, Workshop on Mathematical Aspects of Transport in Mesoscopic Systems, December 4–7, Dublin Institute for Advanced Studies, School of Theoretical Physics, Ireland, December 5.

149. C. Patz, *Hamiltonian passage from many-particle systems to PDEs*, 2 talks, BMS Summer School 2008: Mathematics of Multiscale Phenomena, Berlin Mathematical School/Freie Universität Berlin, Fachbereich Mathematik und Informatik, September 1–12.

150. P. Philip, *Optimal control of conductive-radiative temperature fields generated via electromagnetic heating*, Workshop "Optimal Control of Coupled Systems of PDE", March 2–7, Mathematisches Forschungsinstitut Oberwolfach, March 6.

151. M. Pietrzyk, *On the multisymplectic integrator for the generalized short pulse equation*, 40th Symposium on Mathematical Physics "Geometry & Quanta", June 25–28, Nicolaus Copernicus University, Toruń, Poland, June 28.

152. ———, *Short pulse equations and its properties*, Gdańsk University of Technology, Department of Theoretical Physics and Quantum Information, Poland, July 1.

153. ———, *The short pulse equation: Few-cycle optical pulses beyond the slowly varying envelope approximation*, University of Tartu, Institute of Physics, Estonia, October 8.

154. J. Polzehl, *New developments in structural adaptive smoothing: Images, fMRI and DWI*, University of Tromsoe, Norway, May 27.

155. ———, *Structural adaptive smoothing using the propagation-separation approach*, University of Chicago, Department of Statistics, USA, September 3.

156. ———, *Smoothing fMRI and DWI data using the propagation-separation approach*, University of Utah, Computing and Scientific Imaging Institute, Salt Lake City, USA, September 11.

157. ———, *Structural adaptive smoothing in diffusion tensor imaging*, Workshop on "Locally Adaptive Filters in Signal and Image Processing", November 24–26, EURANDOM, Eindhoven, The Netherlands, November 25.

158. P.N. Racec, *Electrical transport through quantum systems with non-separable scattering potential*, University of Iceland, Science Institute, Reykjavik, June 20.

159. P.N. Racec, *Quantum transport in cylindrical nanowire heterostructures*, Workshop on Mathematical Aspects of Transport in Mesoscopic Systems, December 4–7, Dublin Institute for Advanced Studies, School of Theoretical Physics, Ireland, December 6.

160. A. Rathsfeld, *Scatterometry: Inverse problems and optimization of measurements*, University of Tokyo, Department of Mathematical Sciences, Japan, March 6.

161. J. Rehberg, *Hölder continuity for elliptic and parabolic problems*, Analysis-Tag, Technische Universität Darmstadt, Fachbereich Mathematik, November 27.

162. A. Rohde, *Spatially adaptive comparison of multivariate samples via randomization*, Universität Bern, Switzerland, February 20.

163. ———, *Spatially adaptive comparison of multivariate samples via randomization*, Université Paris VI "Pierre et Marie Curie", France, March 10.

164. ———, *Adaptive goodness-of-fit tests based on signed ranks*, Joint Meeting of the Statistical Society of Canada and the Société Française de Statistique, May 25–29, Statistical Society of Canada, Ottawa, May 26.

165. ———, *Confidence sets for the optimal approximating model — Bridging a gap between adaptive point estimation and confidence regions*, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, June 12.

166. ———, *On Talagrand-type concentration inequalities, decoupling techniques and coupling bounds*, Universität Heidelberg, June 19.

167. ———, *Sharp-optimal adjustment for multiple testing in the multivariate two-sample problem*, Universität Göttingen, June 26.

168. ———, *Sharp-optimal adjustment for multiple testing in the multivariate two-sample problem*, Universität Hamburg, July 18.

169. O. Rott, *Numerical solution of a milling model including thermoelastic workpiece effects*, Universität Dortmund, Fachbereich für Mathematik, June 23.

170. ———, *Modeling, analysis and stability of milling processes including workpiece effects*, The European Consortium for Mathematics in Industry (ECMI 2008), June 30 – July 4, University College, London, UK, July 3.

171. ———, *A milling model with thermal effects including the dynamics of machine and workpiece*, 1st International Conference on Process Machine Interactions (PMI 2008), September 3–4, Leibniz Universität Hannover, September 3.

172. K. Sabelfeld, *Turbulent velocity simulation for aeroacoustics problems*, Russian Academy of Sciences, Sobolev Institute of Mathematics, Novosibirsk, January 17.

173. ———, *Randomized spectral modeling of partially homogeneous random fields*, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, August 6.

174. G. Schmidt, *Integral equations for conical diffraction by coated gratings*, Annual International Conference "Days on Diffraction", June 3–6, St. Petersburg, Russia, June 3.

175. ———, *Approximation of pseudodifferential and integral operators*, Conference "Analysis, PDEs and Applications", June 30 – July 3, Rome, Italy, July 3.

176. ———, *Approximation of pseudodifferential and integral operators*, University of Bath, Department of Mathematical Sciences, UK, December 5.

177. J.G.M. SCHOENMAKERS, *Pricing and hedging exotic interest rate derivatives with Monte Carlo simulation*, 6 talks, finance master class ^{TM} workshop, Concentric Italy, Milan, March 19–20.

178. ———, *Holomorphic transforms and affine processes*, Technische Universität Braunschweig, May 20.

179. ———, *Monte Carlo methods for pricing of complex structured callable derivatives*, 2nd International Conference on Numerical Methods for Finance, June 4–5, Institute for Numerical Computation and Analysis, Dublin, Ireland, June 4.

180. ———, *New Monte Carlo methods for pricing high-dimensional callable derivatives*, Conference on Numerical Methods in Finance, June 26–27, Università di Udine, Italy, June 27.

181. ———, *Regression methods for high-dimensional Bermudan derivatives and stochastic control problems*, Conference on Numerical Methods for American and Bermudan Options, October 17–18, Wolfgang Pauli Institute (WPI), Fakultät für Mathematik, Vienna, Austria, October 17.

182. ———, *Holomorphic transforms with application to affine processes*, 2nd Meeting in the winter semester 2008/2009 of the Research Seminar "Stochastic Analysis and Stochastics of Financial Markets", Technische Universität Berlin, November 6.

183. H. SI, *Constrained Delaunay triangulations and algorithms*, Institut National de Recherche en Informatique et en Automatique – Sophia Antipolis, Le Chesnay, France, March 12.

184. H. SI, *Three dimensional mesh generation, from theory to practice*, University of Basel, Department of Computer Science and Department of Mathematics, Switzerland, May 23.

185. V. SPOKOINY, *Modern nonparametric statistics (block lecture)*, 4 talks, Ecole Nationale de la Statistique et de l'Analyse de l'Information, Rennes, France, February 4–8.

186. ———, *Local parametric time series modeling*, Mini-workshop "Time Series with Sudden Structural Changes", February 24 – March 1, Mathematisches Forschungsinstitut Oberwolfach, February 26.

187. ———, *Local change point detection*, Mini-workshop "Time Series with Sudden Structural Changes", February 24 – March 1, Mathematisches Forschungsinstitut Oberwolfach, February 29.

188. ———, *Modern nonparametric statistics (block lecture)*, 3 talks, Université Catholique de Louvain, Louvaine-la-Neuve, Belgium, March 4–14.

189. ———, *Modern nonparametric statistics (block lecture)*, 3 talks, University of Chicago, USA, March 31 – April 11.

190. ———, *Local parametric modeling for nonstationary time series*, Northwestern University, Chicago, USA, April 8.

191. ———, *Adaptive estimation of time-inhomogeneous financial time series*, Workshop on Finance and Statistics, Stevanovich Center for Financial Mathematics, Chicago, USA, April 10.

192. ———, *Foundations and applications of modern nonparametric statistics (block lecture)*, 3 talks, Graduate School "Mathematics and Practice", Technische Universität Kaiserslautern/Fraunhofer Institut für Techno- und Wirtschaftsmathematik, May 15–16.

193. ———, *Local parametric estimation*, London School of Economics, UK, May 21.

194. ———, *Local parametric modeling of nonstationary time series*, International Workshop on Recent Advances in Time Series Analysis, June 8–11, University of Cyprus, Department of Mathematics and Statistics, Protaras, June 11.

195. ———, *Structure adaptive methods in image denoising*, 2008 International Workshop on Local and Non-Local Approximation in Image Processing (LNLA 2008), August 22–24, Tampere International Center for Signal Processing, Lausanne, Switzerland, August 24.

196. ———, *Foundations and applications of modern nonparametric statistics (block lecture)*, 3 talks, Research Training Group Statistical Modelling, Universität Dortmund, September 24–25.

197. ———, *Adaptive local parametric estimation*, 16th Annual Meeting of the Belgian Statistical Society, October 15–17, Facultés Universitaires Notre-Dame de la Paix, Département de Mathématique, Wépion-Namur, Belgium, October 17.

198. ———, *Adaptive local parametric estimation*, Statistisches Kolloquium, Heinrich-Heine-Universität Düsseldorf, December 1.

199. ———, *Modern parametric statistics*, Rencontres de Statistiques Mathématiques 8, December 15–19, Centre International de Rencontres Mathématiques, Université Aix-Marseille 1, Marseille, France, December 18.

200. J. Sprekels, *Oscillating thin elastoplastic bodies: Dimensional reduction, hysteresis operators, existence results*, Seminar Partial Differential Equations: Models and Applications, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, May 20.

201. ———, *Problems in the industrial growth of semiconductor crystals: Radiative heat transfer, convection, magnetic fields and free boundaries*, The Legacy of John Crank – Developments in Time Dependent PDE's, Diffusion and Free Boundary Problems, July 9–11, Brunel University, Uxbridge, UK, July 10.

202. ———, *Oscillating elastoplastic bodies: Dimensional reduction, hysteresis operators, existence results*, Direct, Inverse and Control Problems for PDE's (DICOP 08), September 22–26, Cortona, Italy, September 22.

203. A. Steinbrecher, *Optimal control of robot guided laser material treatment*, The European Consortium for Mathematics in Industry (ECMI 2008), June 30 – July 4, University College, London, UK, July 3.

204. K. Tabelow, *Strukturadaptive Bild- und Signalverarbeitung*, Workshop of Matheon with Siemens AG (Health Care Sector) in cooperation with Center of Knowledge Interchange (CKI) of Technische Universität (TU) Berlin and Siemens AG, TU Berlin, July 8.

205. A.G. Vladimirov, *Mode-locking in monolithic semiconductor lasers*, University College Cork, Tyndall National Institute, Ireland, March 12.

206. ———, *Bifurcation analysis of a model of passively mode-locked quantum dot laser*, SPIE Photonics Europe Conference, April 7–10, Strasbourg, France, April 8.

207. ———, *Delay differential models of passively mode-locked quantum dot lasers*, Laser Optics 2008, June 23–28, St. Petersburg, Russia, June 25.

208. B. Wagner, *On the wavelength of the contact-line instability of dewetting fronts*, Frontiers in Applied and Computational Mathematics (FACM), May 19–21, New Jersey Institute of Technology, Newark, USA, May 19.

209. ———, *DFG Research Center* MATHEON *and its competences related to the energy sector*, Workshop with Vattenfall Research and Development AG, Technische Universität Berlin, Innovation Centre Energy, June 27.

210. ———, *Patterns in dewetting liquid films: Intermediate and late phases*, Summer Program "Geometrical Singularities and Singular Geometries", July 14–25, University of Minnesota, Institute for Mathematics and Its Applications, USA, July 18.

211. ———, *Coarsening dynamics of slipping droplets*, Conference on Similarity: Generalizations, Applications and Open Problems, August 11–15, University of British Columbia, Vancouver, Canada, August 14.

212. W. Wagner, *Explosion properties of random fragmentation models*, Workshop "Coagulation et Fragmentation Stochastiques", April 15–18, Université Paris VI, Laboratoire de Probabilités, France, April 16.

213. ———, *Introduction to Markov jump processes*, Università di Catania, Dipartimento di Matematica e Informatica, Italy, May 7.

214. ———, *Explosion properties of random fragmentation models*, Università di Catania, Dipartimento di Matematica e Informatica, Italy, May 8.

215. A. Weiss, *Limit order books and optimal portfolio liquidation*, Summer School 2008 Pro * Doc/IRTG Berlin-Zürich "Stochastic Models of Complex Processes", July 21–25, Disentis, Switzerland, July 22.

216. M. Wolfrum, *Delay-differential equations with large delay*, Seminar of the Working Group "Dynamische Systeme", Universität Hamburg, Department Mathematik, January 16.

217. ———, *The Eckhaus scenario in delay-differential equations with large delay*, Workshop "Dynamics of Patterns", December 14–20, Mathematisches Forschungsinstitut Oberwolfach, December 19.

218. S. Yanchuk, *Destabilization in chains of coupled oscillators*, Seminar of Work Group "Neuromodulation", Forschungszentrum Jülich, Institut für Neurowissenschaften und Biophysik, Teilinstitut Medizin, April 29.

219. X. Yao, *Metastability: The potential theoretical methods and its applications*, Peking University, School of Mathematical Sciences, China, June 5.

220. ———, *Random dynamics on the graphical structures*, Tsinghua University of Beijing, Department of Mathematics, China, June 18.

A.8.2 Talks for a More General Public

1. W. Dreyer, *Mathematik und Glück*, Interdisciplinary lecture series "Über das Glück", Universität Erfurt, December 9.

2. M. Ehrhardt, *Die Mathematik des Freiwurfs beim Basketball — Das Geheimnis des Korberfolges*, German "Year of Mathematics 2008", Oberstufenzentrum Wirtschaft und Sozialversicherung, Berlin-Köpenick, March 13.

3. ———, *Die Mathematik des Freiwurfs beim Basketball — Das Geheimnis des Korberfolges*, Wilhelm-von-Siemens-Gymnasium, Berlin, April 15.

4. ———, *Chaos in Liebesaffären*, 13. Berliner Tag der Mathematik (13th Berlin Day of Mathematics), Freie Universität Berlin, April 26.

5. ———, *Chaos in Liebesaffären*, Käthe-Kollwitz-Schule, Berlin, June 25.

6. ———, *Die optimale Flanke oder wie berechne ich die richtige Flugkurve?*, URANIA, Berlin, June 27.

7. ———, *Chaos in Liebesaffären*, Rudolf-Virchow-Oberschule, Berlin, July 4.

8. ———, *Die Mathematik des Freiwurfs beim Basketball — Das Geheimnis des Korberfolges*, Johann-Gottfried-Herder-Gymnasium, Berlin, July 8.

9. ———, *Die Mathematik des Klimawandels — Ein globales CO_2-Modell*, Lise-Meitner-Schule, Berlin, September 8.

10. ———, *Die Mathematik des Klimawandels — Ein globales CO_2-Modell*, URANIA, Berlin, October 14.

11. K. Gärtner, *Lineare Gleichungssysteme lösen, kann das Spaß machen?*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2008, WIAS, June 14.

12. J. Kampen, *Quantenrechner und ihre mathematischen Grundlagen*, German "Year of Mathematics 2008", Frankfurter Salon, Frankfurt am Main, February 14.

13. Ch. Kraus, *Alles geht kaputt? Entmischungsphänomene, Schädigungsprozesse und Rissbildung in Natur und Technik*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2008, WIAS, June 14.

14. P. Krejčí, *The mathematics of memory*, Berlin-Brandenburger Humboldt-Dialog, Alexander von Humboldt-Stiftung, Berlin, November 19.

15. Ch. Meyer, *Auf der Suche nach dem Optimum — Was kommt nach der Kurvendiskussion?*, Raabe-Gymnasium, Braunschweig, February 1.

16. ———, *Auf der Suche nach dem Optimum — Wozu braucht man die Kurvendiskussion?*, 13. Berliner Tag der Mathematik (13th Berlin Day of Mathematics), Freie Universität Berlin, April 26.
17. ———, *Auf der Suche nach dem Optimum — Was kommt nach der Kurvendiskussion?*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2008, WIAS, June 14.
18. G. Reinhardt, *Was ist "digital" beim digitalen Fernsehen*, 13. Berliner Tag der Mathematik (13th Berlin Day of Mathematics), Freie Universität Berlin, April 26.
19. F. Schmid, *Schon einmal in die Zukunft geschaut?*, 13. Berliner Tag der Mathematik (13th Berlin Day of Mathematics), Freie Universität Berlin, April 26.
20. J. Sprekels, *DFG-Forschungszentrum* Matheon*: Mathematik — Hochleistungsmikroskop und virtuelles Labor für Schlüsseltechnologien*, Annual Meeting of the Leibniz Association, November 26–28, Magdeburg, November 26.
21. A. Steinbrecher, *MATLAB — Eine Einführung*, Pupils' Workshop of Matheon and BMBF, Technische Universität Berlin, January 22–23.
22. A. Weiss, *Money, money, money: Aktionär und trotzdem arm?*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2008, WIAS, June 14.
23. M. Wolfrum, *Wege ins Chaos*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2008, WIAS, June 14.

A.8.3 Posters

1. M. Ehrhardt, O. Gloger, Th. Dietrich, O. Hellwich, K. Graf, E. Nagel, *Level Set Methoden zur Segmentierung von kardiologischen MR-Bildern*, 22. Treffpunkt Medizintechnik: Fortschritte in der medizinischen Bildgebung, Charité, Campus Virchow Klinikum Berlin, May 22.
2. E. Bänsch, H. Berninger, U. Böhm, A. Bronstert, M. Ehrhardt, R. Forster, J. Fuhrmann, R. Klein, R. Kornhuber, A. Linke, A. Owinoh, J. Volkholz, *Pakt für Forschung und Innovation: Das Forschungsnetzwerk "Gekoppelte Strömungsprozesse in Energie- und Umweltforschung"*, Show of the Leibniz Association "Exzellenz durch Vernetzung. Kooperationsprojekte der deutschen Wissenschaftsorganisationen mit Hochschulen im Pakt für Forschung und Innovation", Berlin, November 12.
3. A. Fiebach, J. Fuhrmann, *Some reaction diffusion problems in semiconductor device fabrication*, Workshop on PDE approximations in Fast reaction – Slow diffusion scenarios, Leiden, The Netherlands, November 10–14.
4. J. Fuhrmann, *Berechnendes Denken: Zusammenhänge verstehen durch Modellierung*, BMBF Status Seminar "Formel M: Mathematik für Innovation und Energieforschung", Duisburg, October 26–28.
5. K. Hoke, *Numerical treatment of the Kohn–Sham system for semiconductor devices*, Workshop on Mathematical Aspects of Transport in Mesoscopic Systems, Dublin, Ireland, December 4–7.
6. E. Holzbecher, H. Zhao, J. Fuhrmann, A. Linke, H. Langmach, *Numerical investigation of thin layer flow cells*, 4th Gerischer Symposium "Electrochemistry with Spatial and Temporal Resultion", Berlin, June 25–27.
7. W. Bleck, D. Hömberg, Ch. Keul, U. Prahl, P. Suwanpinij, N. Togobytska, *Simulation, Optimierung und Regelung von Gefügebildung und mechanischen Eigenschaften beim Warmwalzen von Mehrphasenstählen*, Workshop "MEFORM 2008: Simulation von Umformprozessen", Freiberg, March 26–28.
8. M. Korzec, *Stationary solutions and coarsening of a driven Cahn–Hilliard-type equation*, Summer Program "Geometrical Singularities and Singular Geometries" of the Institute for Mathematics and Its Applications, Minneapolis, USA, July 14–25.

9. C. Krüger, A. Demircan, G. Stibenz, N. Zhavoronkov, G. Steinmeyer, *Asymptotic pulse shapes and pulse self-compression in femtosecond filaments*, UP 2008: XVI Conference on Ultrafast Phenomena, Stresa, Italy, June 9–13.
10. ———, *Asymptotic pulse shapes in filamentary propagation of femtosecond pulses and self-compression*, CLEO/QUELS 2008: Conference on Lasers and Electro-Optics/Quantum Electronics and Laser Science Conference, San Jose, USA, May 4–9.
11. M. Pietrzyk, I. Kanattšikow, *Multisymplectic integrators in nonlinear optics*, PHOTON08: Conference in Optics and Photonics, Edinburgh, UK, August 26–29.
12. P.N. Racec, *Modelling of nanowire transistors in Landauer–Büttiker formalism*, Spring Meeting of the Condensed Matter Division of the Deutsche Physikalische Gesellschaft, Berlin, February 25–29.
13. K. Tabelow, *Structure adaptive smoothing medical images*, 22. Treffpunkt Medizintechnik: Fortschritte in der medizinischen Bildgebung, Charité, Campus Virchow Klinikum Berlin, May 22.

A.8.4 Contributions to Exhibitions

1. F. Anker, I. Bremer, M. Kiebinger, T. Köhler, *Virtuelle Realität in der Produktionsplanung*, Wissenschaftssommer (Summer of Science) 2008, June 28 – July 4, Leipzig.

A.9 Visits to other Institutions[5]

1. O. Zindy, Université Henri Poincaré, Faculté des Sciences et Techniques, Nancy, France, January 29 – February 3.
2. ———, University of Cambridge, Faculty of Mathematics, UK, February 4–10.
3. L.-P. Arguin, Stanford University, Department of Mathematics, USA, February 8–13.
4. ———, New York University, Courant Institute of Mathematical Sciences, USA, February 14–18.
5. ———, Universität Zürich, Mathematisch-naturwissenschaftliche Fakultät, Switzerland, March 4–8.
6. U. Bandelow, University of Washington, Department of Applied Mathematics, Seattle, USA, October 13–17.
7. D. Belomestny, Technische Universität Wien, Institut für Wirtschaftsmathematik, Austria, September 22–26.
8. A. Bianchi, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, April 24 – May 25.
9. A. Bovier, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, December 20, 2007 – January 6, 2008.
10. ———, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, Israel, May 12–25.
11. M. Ehrhardt, Comenius University, Department of Applied Mathematics and Statistics, Bratislava, Slovakia, June 2–6.
12. ———, Université des Sciences et Technologies de Lille, Laboratoire Paul Painlevé, INRIA SIMPAF Team, France, September 22–28.
13. J. Ehrt, Centrum voor Wiskunde & Informatica, Amsterdam, The Netherlands, August 4 – October 31.
14. J. Elschner, University of Tokyo, Department of Mathematical Sciences, Japan, February 18 – March 7.
15. P. Ferrari, California Institute of Technology, CALTECH, Department of Mathematics, Pasadena, USA, February 9–23.
16. ———, Université Catholique de Louvain, Faculté des Sciences, Belgium, May 19–24.
17. R. Henrion, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, August 25–28.
18. D. Hömberg, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, February 11–15.
19. D. Horn, ALSTOM (Switzerland) Ltd., Baden, Switzerland, June 3–6.
20. H.-Chr. Kaiser, Université de Rennes 1, Institut de Recherche Mathématique de Rennes, France, May 18–24.
21. I. Kanattšikow, Gdańsk University of Technology, Theoretical Physics and Quantum Informatics Department, Poland, June 30 – July 4.
22. ———, University of Leeds, Department of Mathematics, UK, September 3–7.
23. ———, University of Trieste, Department of Theoretical Physics, Italy, November 21 – December 2.
24. D. Knees, Charles University, Mathematical Institute, Prague, Czech Republic, March 5–8.

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

25. Th. Koprucki, Université de Rennes, Institut de Recherche Mathématique de Rennes, France, May 19–23.
26. P. Krejčí, Fudan University, School of Mathematical Sciences, Shanghai, China, April 30 – May 30.
27. ———, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, November 23–30.
28. C. Krüger, Max-Planck-Institut für Physik komplexer Systeme, Dresden, March 31 – April 4.
29. A. Linke, Université de Marne-la-Vallée, Département de Mathématiques, Champs-sur-Marne, France, August 18–22.
30. P. Mathé, Austrian Academy of Sciences, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, October 25 – November 21.
31. Ch. Meyer, Technische Universität Chemnitz, Fakultät für Mathematik, June 24–27.
32. ———, Universität der Bundeswehr München, Institut für Mathematik und Bauinformatik, July 8–11.
33. ———, Technische Universität Chemnitz, Fakultät für Mathematik, October 27–31.
34. A. Mielke, Charles University/Jindrich Nečas Center for Mathematical Modeling, Prague, Czech Republic, February 25 – March 16.
35. ———, Charles University/Jindrich Nečas Center for Mathematical Modeling, Prague, Czech Republic, November 10–15.
36. H. Neidhardt, Centre National de la Recherche Scientifique Luminy, Centre de Physique Théorique, Marseille, France, October 12–25.
37. A. Petrov, C.I.M.E. — Centro Internazionale Matematico Estivo, Cetraro (Cosenza), Italy, June 22–26.
38. M. Pietrzyk, Gdańsk University of Technology, Theoretical Physics and Quantum Informatics Department, Poland, June 30 – July 4.
39. J. Polzehl, University of Tromsoe, Institute of Mathematics and Statistics, Norway, May 26–30.
40. ———, University of Minnesota, School of Statistics, Minneapolis, USA, September 1–17.
41. P.N. Racec, University of Iceland, Science Institute, Reykjavik, June 15–22.
42. A. Rathsfeld, University of Tokyo, Department of Mathematical Sciences, Japan, February 25 – March 7.
43. A. Rohde, Universität Bern, Institut für Mathematische Statistik und Versicherungslehre, Switzerland, February 17–29.
44. ———, LS CREST Laboratoire de Statistique du Crest, Malakoff, France, March 3–31.
45. ———, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, May 5–16.
46. ———, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, June 9–15.
47. ———, Universität Heidelberg, Institut für Angewandte Mathematik, August 7–15.
48. K. Sabelfeld, Russian Academy of Sciences, Sobolev Institute of Mathematics, Novosibirsk, December 28, 2007 – January 24, 2008.
49. ———, Russian Academy of Sciences, Institute for Mathematical Modelling, Moscow, April 8 – May 7.
50. ———, Universität Erlangen-Nürnberg, Institute of Applied Mathematics, May 25 – June 4.
51. ———, Russian Academy of Sciences, Department of Mathematics, Novosibirsk, August 4 – September 12.
52. F. Schmid, Hochleistungsrechenzentrum Stuttgart — HLRS, October 6–10.
53. G. Schmidt, University of Liverpool, Department of Mathematical Sciences, UK, December 1–11.
54. N. Serdyukova, Universität Linz, Department of Knowledge-Based Mathematical Systems, Austria, September 16–20.

55. H. Si, Institut National de Recherche en Informatique et Automatique – Sophia Antipolis, Le Chesnay, France, March 11–14.
56. V. Spokoiny, Université Sophia Antipolis, Faculté des Sciences, Nice, France, June 24–27.
57. J. Sprekels, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, May 16–21.
58. K. Tabelow, Cornell University New York, Weill Medical College, USA, March 17–26.
59. V.Z. Tronciu, Universitat de les Illes Balears, Instituto de Física Interdisciplinar y Sistemas Complejos (CSIC-UIB), Palma de Mallorca, Spain, October 23–26.
60. A.G. Vladimirov, Free University of Brussels (ULB), Theoretical Nonlinear Optics Group, Belgium, February 4–18.
61. ———, University College Cork, School of Mathematical Sciences, Ireland, March 6–18.
62. ———, Ben Gurion University of the Negev, Department of Mathematics, Beer-Sheva, Israel, April 14–29.
63. ———, Vavilov State Optical Institute, Research Institute for Laser Physics, St. Petersburg, Russia, June 30 – July 4.
64. W. Wagner, Università di Catania, Dipartimento di Matematica e Informatica, Italy, May 5–9.
65. ———, Cambridge University, Department of Chemical Engineering, UK, May 26–29.
66. ———, Universität des Saarlandes, Fachbereich Mathematik, Saarbrücken, October 7–10.
67. M. Wolfrum, Technical University of Lodz, Faculty of Mechanical Engineering, Division of Dynamics, Poland, March 2–7.
68. S. Yanchuk, Technical University of Lodz, Faculty of Mechanical Engineering, Division of Dynamics, Poland, March 2–7.
69. X. Yao, Peking University, School of Mathematical Sciences, China, May 28 – July 1.

A.10 Academic Teaching[6]

Winter Semester 2007/2008

1. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS.
2. D. Belomestny, *Statistik der Finanzmärkte* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
3. A. Bovier, *Wahrscheinlichkeitstheorie IV – BMS Basic Course Stochastic Processes III* (lecture), Technische Universität Berlin, 2 SWS.
4. ———, *Oberseminar biologische Modelle und statistische Mechanik* (senior seminar), Technische Universität Berlin, 2 SWS.
5. ———, *Wahrscheinlichkeitstheorie* (practice), Technische Universität Berlin, 2 SWS.
6. A. Bovier, 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.
7. W. Dreyer, *Tensoranalysis* (lecture), Technische Universität Berlin, Institut für Mechanik, 4 SWS.
8. P. Ferrari, *Random Matrices and Related Problems* (lecture), Technische Universität Berlin, 3 SWS.
9. E. Giacomini, W. Härdle, *Statistical Tools in Finance and Insurance* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
10. A. Glitzky, *Einführung in die Kontrolltheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
11. J.A. Griepentrog, *Funktionenräume für nichtglatte parabolische Probleme* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
12. R. Henrion, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
13. R. Henrion, W. Römisch, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
14. E. Holzbecher, *Grundwassermodellierung II* (lecture), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
15. ———, *Grundwassermodellierung II* (practice), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
16. Ch. Meyer, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
17. A. Mielke, *Ausgewählte Themen der Variationsrechnung* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
18. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS.
19. V. Spokoiny, *Nichtparametrische Methoden und ihre Anwendungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
20. V. Spokoiny, W. Härdle, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
21. J. Sprekels, *Höhere Analysis I (Funktionalanalysis)/BMS Basic Course "Functional Analysis"* (lecture), Humboldt-Universität zu Berlin, 4 SWS.

[6] SWS = semester periods per week

22. 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.
23. K. Tabelow, *Mathematik* (seminar), Deutsches Herzzentrum Berlin, Akademie für Kardiotechnik, 2 SWS.
24. M. Wolfrum, B. Fiedler, S. Liebscher, *Nichtlineare Dynamik* (senior seminar), WIAS/Freie Universität Berlin, 2 SWS.

Summer Semester 2008

1. U. Bandelow, *Nichtlineare Effekte in Halbleiterlasern und Optischen Fasern* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
2. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS.
3. M. Birkner, *Angewandte Stochastik* (lecture), Universität Bonn, 4 SWS.
4. ———, *Kombinatorische Stochastische Prozesse* (seminar), Universität Bonn, 2 SWS.
5. ———, *Angewandte Stochastik* (practice), Universität Bonn, 2 SWS.
6. A. Bovier, H. Föllmer, P. Imkeller, U. Küchler, J.-D. Deuschel, J. Gärtner, M. Scheutzow, A. Schied, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Technische Universität Berlin, 2 SWS.
7. M. Ehrhardt, *Level-Set-Methoden mit Anwendungen in der medizinischen Bildverarbeitung* (seminar), Technische Universität Berlin, 2 SWS.
8. ———, *Mit Mathematik Kriminalfälle lösen* (seminar), Technische Universität Berlin, 2 SWS.
9. J.A. Griepentrog, *Regularitätstheorie für nichtglatte parabolische Probleme* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
10. R. Henrion, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
11. R. Henrion, W. Römisch, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
12. E. Holzbecher, *Geothermics Modeling* (lecture), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
13. ———, *Geothermics Modeling* (practice), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
14. D. Hömberg, *Optimalsteuerung bei partiellen Differentialgleichungen* (lecture), Technische Universität Berlin, 4 SWS.
15. O. Klein, *Optimale Steuerung partieller Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
16. P. Mathé, *Inverse Probleme, Lehrgebiet: Mathematik, Numerische Analysis* (lecture), Technische Universität Chemnitz, 2 SWS.
17. Ch. Meyer, *Analysis II für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS.
18. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS.
19. V. Spokoiny, *Modern Methods in Applied Stochastics and Nonparametric Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
20. V. Spokoiny, W. Härdle, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.

21. J. Sprekels, *Höhere Mathematik II (Partielle Differentialgleichungen)/BMS Basic Course "Partial Differential Equations"* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
22. 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.
23. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
24. M. Wolfrum, B. Fiedler, S. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS/Freie Universität Berlin, 2 SWS.

Winter Semester 2008/2009

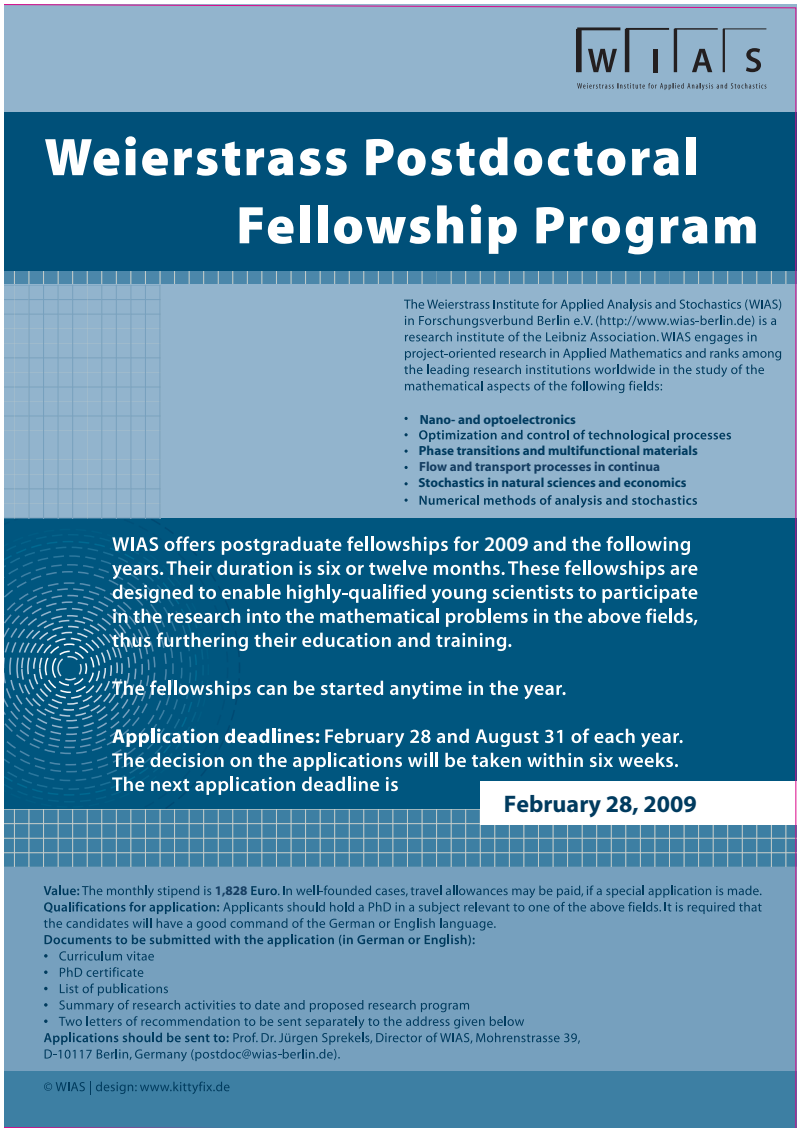
1. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS.
2. D. Belomestny, W. Härdle, O. Okhrin, *Statistical Tools in Finance and Insurance* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
3. M. Ehrhardt, *Asymptotische Analysis* (lecture), Technische Universität Berlin, 2 SWS.
4. ———, *Transport in porösen Medien — Modellierung, Analysis und Numerik* (seminar), Technische Universität Berlin, 2 SWS.
5. ———, *Asymptotische Analysis* (practice), Technische Universität Berlin, 1 SWS.
6. J. Fuhrmann, *Integraltransformation und partielle Differentialgleichungen* (lecture), Technische Universität Berlin, 2 SWS.
7. A. Glitzky, *Grundlagen der Kontrolltheorie und optimalen Steuerung/BMS Advanced Course "Introduction to Control Theory and Optimal Control"* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
8. D. Hömberg, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
9. O. Klein, *Analytische Eigenschaften von Hysterese-Operatoren; Evolutionsgleichungen mit Hysterese-Operatoren* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
10. D. Knees, *Allgemeine Variationsmethoden I/BMS Advanced Course "General Variational Methods I"* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
11. M. Korzec, *Lineare Algebra für Ingenieure* (practice), Technische Universität Berlin, 4 SWS.
12. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS.
13. V. Spokoiny, W. Härdle, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
14. V. Spokoiny, M. Reiss, *Nichtparametrische Statistik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
15. 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.
16. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
17. N. Togobytska, *Nichtlineare Optimierung* (practice), Technische Universität Berlin, 2 SWS.
18. M. Wolfrum, B. Fiedler, S. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS/Freie Universität Berlin, 2 SWS.

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 main fields of the institute 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.

In 2008, Dr. Giada Basile (Université de Paris-Dauphine, France, and Università degli Studi di Firenze, Italy), Dr. Olivier Lopez (Ecole Nationale de la Statistique et de l'Analyse de l'Information, Rennes, France), Dr. Oleh Omel'chenko (National Academy of Sciences of Ukraine, Kiev), Dr. Hao Wu (Fudan University, Shanghai, China), and Dr. Olivier Zindy (Université Paris VI, France) worked as fellowship holders at WIAS.



A.12 Visiting Scientists[7]

A.12.1 Guests

1. F. Bauer, Johannes Kepler Universität Linz, Institut für Wissensbasierte Mathematische Systeme, Austria, February 4–10.
2. A.B. Bhattacherjee, University of Delhi, Atma Ram Sanatan Dharm College, India, October 1–22.
3. L. Birgé, Université Paris VI, Laboratoire de Probabilités, France, May 18–22.
4. J. Brasche, Technische Universität Clausthal, Institut für Mathematik, April 21–24.
5. M. Brokate, Technische Universität München, Zentrum Mathematik, February 4–8.
6. J. Cerný, Eidgenössische Technische Hochschule Zürich, Department of Mathematics, Switzerland, February 2–8.
7. N. Champagnat, Institut National de Recherche en Informatique et Automatique – Sophia Antipolis, France, April 6–11.
8. K. Chełminski, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, June 16 – July 14.
9. R. Čiegis, Vilnius Gediminas Technical University, Department of Mathematical Modeling, Lithuania, October 13 – November 7.
10. P. Colli, Università di Pavia, Dipartimento di Matematica, Italy, May 24 – June 1.
11. P. Contucci, Università di Bologna, Dipartimento di Matematica, Italy, June 15 – July 12.
12. A. Dalalyan, Université Paris VI, Laboratoire de Probabilités, France, November 24–27.
13. E. Di Stefano, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, May 31 – June 30.
14. J. Dupačová, Charles University, Department of Probability and Mathematical Statistics, Prague, Czech Republic, January 9–13.
15. A. Egorov, National Academy of Sciences of Belarus, Institute of Mathematics, Minsk, October 2 – December 1.
16. S.M. Ermakov, University of St. Petersburg, Faculty of Mathematics and Mechanics, Russia, October 25 – November 2.
17. P. Evans, Humboldt-Universität zu Berlin, Institut für Mathematik, July 27, 2006 – December 31, 2009.
18. R. Eymard, Université Paris Est, Département de Mathématiques, Marne-la-Vallée, France, February 10–16.
19. J. Giannoulis, Technische Universität München, Zentrum Mathematik, June 30 – July 9.
20. C. Giardina, Technical University of Eindhoven, Department of Mathematics and Computer Science, The Netherlands, July 1–12.
21. Y. Golubev, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, April 21 – May 16.
22. L.I. Goray, Russian Academy of Sciences, Institute for Analytical Instrumentation, St. Petersburg, October 26 – November 2.

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

23. R. Griesse, Technische Universität Chemnitz, Fakultät für Mathematik, August 11 – September 6.
24. R. Haller-Dintelmann, Technische Universität Darmstadt, Fachbereich Mathematik, February 11–29.
25. S. Heinz, University of Wyoming, Department of Mathematics, Laramie, USA, June 26 – July 3.
26. M. Herrmann, University of Oxford, Mathematical Institute, UK, September 7–13.
27. J. Horowitz, Northwestern University, Department of Economics, Evanston, Illinois, USA, December 4–13.
28. G.C. Hsiao, University of Delaware, Department of Mathematical Sciences, Newark, USA, July 2 – August 1.
29. O. Iliev, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern, June 23–27.
30. D. Ioffe, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, July 31 – August 31.
31. A. Juditsky, Université Joseph Fourier Grenoble I, Laboratoire de Modélisation et Calcul, France, December 21–26.
32. T. Kapitaniak, Technical University of Łodz, Division of Dynamics, Poland, May 10–19.
33. ———, November 10–20.
34. P.L. Kaufmann, University of Sao Paulo, Institute of Mathematics and Statistics, Brazil, February 18–22.
35. ———, April 21–25.
36. M. Keller-Ressel, Technische Universität Wien, Institut für Wirtschaftsmathematik, Austria, January 14–18.
37. S.-J. Kimmerle, Humboldt-Universität zu Berlin, Institut für Mathematik, January 1, 2008 – May 31, 2010.
38. N. Kistler, École Normale Supérieure de Lyon, Unité de Mathématiques Pures et Appliquées, France, June 30 – July 5.
39. J. Kopfová, Silesian University in Opava, Mathematical Institute, Czech Republic, February 4–8.
40. T. Kozubskaya, Russian Academy of Sciences, Institute for Mathematical Modelling, Moscow, May 26 – June 9.
41. M. Kraft, University of Cambridge, Department of Chemical Engineering, UK, October 13 – November 14.
42. A. Kruger, University of Ballarat, School of Information Technology and Mathematical Sciences, Australia, September 17–21.
43. K. Krumbiegel, Universität Duisburg-Essen, Fachbereich Mathematik, March 16–21.
44. O. Kurbanmuradov, Turkmen State University, Physics and Mathematics Research Center, Ashkhabad, October 1 – December 1.
45. Ch. Lechner, Vienna, Austria, November 30 – December 6.
46. O. Lepski, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, April 21 – May 4.
47. ———, October 26 – November 3.
48. Y. Liu, Peking University, Department of Mathematics, China, January 16 – February 16.
49. M.M. Malamud, Donetsk National University, Department of Mathematics, Ukraine, April 23–29.
50. ———, December 8–17.
51. P.A. Mayer, Technische Universität Graz, Institut für Optimierung und diskrete Mathematik, Austria, March 25 – April 4.

52. H. Michinel, University of Vigo, Faculty of Sciences, Ourense, Spain, March 1–31.
53. G. Milstein, University of Leicester, Department of Mathematics, UK, October 20 – December 20.
54. V. Moldoveanu, National Institute of Materials Physics, Laboratory of Low Dimensional Systems, Bucharest, Romania, December 17–23.
55. A. Münch, University of Nottingham, School of Mathematical Sciences, UK, February 13–17.
56. ———, September 2–7.
57. O. Muscato, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, February 4–8.
58. ———, August 24–31.
59. G. Nenciu, Romanian Academy, Institute of Mathematics, Bucharest, September 20 – October 5.
60. S. O'Brien, Tyndall National Institute, Cork, Ireland, December 16–19.
61. S. Olla, Université Paris Dauphine, Centre de Recherche en Mathématiques de la Décision, France, January 28 – February 3.
62. J. Outrata, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, October 26 – November 1.
63. ———, November 30 – December 12.
64. V. Panov, StatSoft Russia, Moscow, June 15–22.
65. L. Paoli, Université de Saint-Etienne, Laboratoire de Mathématiques, France, January 7 – February 7.
66. ———, June 1–14.
67. V. Patilea, Institut National des Sciences Appliquées (INSA) de Rennes, Centre des Mathématiques, France, May 1–8.
68. S. Peché, Institut Fourier, Laboratoire de Mathématiques, Saint Martin d'Hères, France, July 21–25.
69. P. Perlikowski, Technical University of Łodz, Division of Dynamics, Poland, May 10–31.
70. A. Pimenov, University College Cork, Department of Applied Mathematics, Ireland, January 10–27.
71. ———, May 6 – June 7.
72. A. Politi, Consiglio Nazionale delle Ricerche, Istituto dei Sistemi Complessi, Florence, Italy, November 12–20.
73. D. Rachinskii, University College Cork, Department of Applied Mathematics, Ireland, June 12–17.
74. J. Rademacher, Centrum voor Wiskunde & Informatica, Department Modelling, Analysis and Simulation, Amsterdam, The Netherlands, January 14 – February 8.
75. N. Rebrova, Tyndall National Institute, Photonic Device Dynamics Group, Cork, Ireland, December 10, 2008 – January 10, 2009.
76. T. Rees, Oxford University, Computing Laboratory, UK, April 20–25.
77. W. Ring, Karl-Franzens-Universität Graz, Institut für Mathematik, Austria, July 14 – August 8.
78. E. Rocca, Università degli Studi di Milano, Dipartimento di Matematica "F. Enriques", Italy, October 22 – November 14.
79. E. Rohan, University of West Bohemia, Faculty of Applied Sciences, Plzen, Czech Republic, December 2–5.

80. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, January 21 – February 18.
81. ———, June 16 – July 15.
82. ———, August 20 – September 19.
83. D. Rudolf, Friedrich-Schiller-Universität Jena, Mathematisches Institut, May 26–30.
84. A. Scheel, University of Minnesota, School of Mathematics, Minneapolis, USA, March 1 – May 31.
85. O. Schenk, University of Basel, Department of Computer Science, Switzerland, August 4–8.
86. M. Schieck, Technische Universität Chemnitz, Fakultät für Mathematik, March 31 – April 4.
87. F. Schilder, University of Surrey, Department of Mathematics, Guildford, UK, November 30 – December 24.
88. V. Seremet, Agrarian State University, Chisinau, Republic of Moldova, October 14 – November 14.
89. I. Shalimova, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, February 28 – March 28.
90. ———, June 3 – July 2.
91. ———, October 9 – November 8.
92. J. Sokołowski, Université de Nancy I, Laboratoire de Mathématiques, Vandœuvre-lès-Nancy, France, October 19–26.
93. V.A. Solonnikov, Steklov Institute of Mathematics, Petersburg Department, Laboratory of Mathematical Physics, Russia, April 14–19.
94. Ch. Sparber, University of Cambridge, Department of Applied Mathematics and Theoretical Physics, UK, June 30 – July 9.
95. S. Starr, University of Rochester, Department of Mathematics, USA, July 5–12.
96. A. Stefanski, Technical University of Łodz, Division of Dynamics, Poland, May 10–19.
97. ———, November 10–20.
98. M. Tlidi, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, November 16–22.
99. A. Torcini, Consiglio Nazionale delle Ricerche, Istituto dei Sistemi Complessi, Florence, Italy, April 5–28.
100. M. Tretyakov, University of Leicester, Department of Mathematics, UK, December 6–19.
101. K. Trivisa, University of Maryland, Department of Mathematics, College Park, USA, June 22 – July 20.
102. O. Trubitsyna, Biovesta, Med. Akad., Novosibirsk, Russia, May 16 – June 15.
103. D. Turaev, Imperial College London, Department of Mathematics, UK, August 15–30.
104. V. Uchaikin, Ulyanovsk State University, Chair of Theoretical and Mathematical Physics, Russia, May 7 – July 6.
105. E. Verbree, Delft University of Technology, OTB Institute for Housing, Urban and Mobility Studies, The Netherlands, October 15–18.
106. E.A. Viktorov, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, December 1–5.
107. M. Wouts, Université Paris X, Équipe Modal'X, France, March 4–9.
108. M. Yamamoto, University of Tokyo, Department of Mathematical Sciences, Japan, April 10 – May 13.
109. ———, September 7–21.

110. Q. Yao, London School of Economics, Department of Statistics, UK, July 8–18.

111. S. Yoshikawa, Ube National College of Technology, Department of Business Administration, Ube, Japan, March 8–18.

112. Ch. Zanini, Università degli Studi di Udine, Dipartimento di Matematica e Informatica, Italy, May 18 – June 7.

113. D. Zeitz, ALSTOM (Switzerland) Ltd., Baden, August 11–22.

A.12.2 Scholarship Holders

1. G. Basile, Université Paris-Dauphine, France, and Università degli Studi di Firenze, Italy, Weierstrass Postdoctoral Fellowship Program, September 1, 2007 – August 31, 2008.
2. O. Lopez, CREST- Ecole Nationale de la Statistique et de l'Analyse de l'Information (ENSAI), Rennes, France, Weierstrass Postdoctoral Fellowship Program, February 1 – July 31.
3. O. Omel'chenko, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, Weierstrass Postdoctoral Fellowship Program, December 1, 2008 – November 30, 2009.
4. L. Panizzi, Scuola Normale Superiore, Pisa, Italy, Fellowship of the Scuola Normale Superiore, January 1 – September 30.
5. L.P. Shilnikov, N.I. Lobachevsky State University of Nizhny Novgorod, Institute for Applied Mathematics and Cybernetics, Humboldt Research Award, January 25 – February 24.
6. H. Wu, Fudan University, School of Mathematical Sciences, Shanghai, China, Weierstrass Postdoctoral Fellowship Program, September 1, 2008 – August 31, 2009.
7. O. Zindy, Université Paris VI, Laboratoire de Probabilités et Modèles Aléatoires, France, Weierstrass Postdoctoral Fellowship Program, September 1, 2007 – August 31, 2008.

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

1. A. Depperschmidt, Technische Universität Berlin, doctoral candidate, January 1, 2004 – July 31, 2008.
2. G. Di Gesu, Technische Universität Berlin, International Research Training Group GRK 1339: "Stochastic Models of Complex Systems and Their Applications", doctoral candidate, May 30, 2007 – May 31, 2010.
3. O. Gloger, Technische Universität Berlin, doctoral candidate, since April 1, 2007.
4. S. Hock, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", doctoral candidate, May 1, 2005 – March 31, 2008.
5. S.-J. Kimmerle, Humboldt-Universität zu Berlin, Institut für Mathematik, DFG Research Center Matheon, subproject C14, doctoral candidate, January 1, 2007 – May 31, 2010.
6. G. Kitavtsev, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", doctoral candidate, January 1, 2007 – April 30, 2009.
7. A. Klimovski, Technische Universität Berlin, doctoral candidate, June 1, 2003 – June 24, 2008.
8. M. Liero, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", doctoral candidate, December 1, 2008 – November 30, 2011.
9. D. Marx, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", doctoral candidate, May 15, 2006 – May 14, 2009.
10. L. Panizzi, Scuola Normale Superiore, Pisa, Italy, doctoral candidate, since October 1.

11. Th. Petzold, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 “Analysis, Numerics, and Optimization of Multiphase Problems”, doctoral candidate, May 1, 2005 – December 31, 2009.
12. A. Pimenov, University College Cork, Department of Applied Mathematics, doctoral candidate, October 1, 2006 – August 31, 2009.
13. Th. Surowiez, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 “Analysis, Numerics, and Optimization of Multiphase Problems”, doctoral candidate, August 1, 2006 – July 31, 2009.
14. M. Thomas, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 “Analysis, Numerics, and Optimization of Multiphase Problems”, doctoral candidate, January 1, 2007 – December 31, 2009.
15. D. Wegner, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 “Analysis, Numerics, and Optimization of Multiphase Problems”, doctoral candidate, May 1, 2005 – December 31, 2008.

A.13 Guest Talks

1. A. Amann, Tyndall National Institute, Cork, Ireland, *Bifurcation analysis for an injected two-mode laser: How to explain a complicated laser with a simple model*, December 4.
2. A. Baranovski, WestLB AG, BU Credit Risk Management, Düsseldorf, *From fitting spread curves to the estimation of default intensities*, June 17.
3. F. Bauer, Johannes Kepler Universität Linz, Institut für Wissensbasierte Mathematische Systeme, Austria, *Choosing regularization parameters in an optimal way without knowing the noise level — Analysis of quasi-optimality*, February 5.
4. M. Belhaq, University Hassan II, Faculty of Sciences, Laboratory of Mechanics, Casablanca, Morocco, *Control of limit cycle and hysteresis suppression in driven self-sustained oscillators*, February 19.
5. N. Ben-Gal, Brown University, Division of Applied Mathematics, Providence, USA, now Freie Universität Berlin, *Asymptotics of grow-up solutions and global attractors of non-dissipative PDEs*, November 11.
6. W.D. Bessler, Ruprecht-Karls-Universität Heidelberg, Interdisziplinäres Zentrum für Wissenschaftliches Rechnen, *Elektrochemie und Transport in Feststoffoxid-Brennstoffzellen*, April 22.
7. A.B. Bhattacherjee, University of Delhi, ARSD College, India, *Matter wave dark solitons in optical superlattices*, October 16.
8. L. Birgé, Université Paris VI, Laboratoire de Probabilités, France, *Model selection for Poisson processes*, May 21.
9. P. Birken, Universität Kassel, AG Analysis und Angewandte Mathematik, *Mathematik in der deutschsprachigen Wikipedia*, October 27.
10. P. Birken, H. Fiebig, Universität Kassel, AG Analysis und Angewandte Mathematik/Wikimedia Deutschland e.V., *Wissen teilen leicht gemacht: Eine kurze Einführung für Wikipedia-Einsteiger*, October 27.
11. T. Bodnar, Europa-Universität Viadrina, Wirtschaftswissenschaftliche Fakultät, Frankfurt (Oder), *On the product of inverse Wishart and normal distributions with applications to discriminant analysis*, July 15.
12. G. Bordyugov, Universität Potsdam, Institut für Physik und Astronomie, *Response functions of spiral waves*, October 28.
13. J. Brasche, Technische Universität Clausthal, Institut für Mathematik, *Approximation of Schrödinger operators by modified point interaction operators*, April 23.
14. O. Burylko, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, *Bifurcations to heteroclinic cycles in phase coupled oscillators*, June 17.
15. L. Cavalier, Université Aix-Marseille 1, Centre de Mathématiques et Informatique, France, *Risk hull method for inverse problems*, April 23.
16. K. Chełminski, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, *Regularity questions in the theory of inelastic deformations*, June 24.
17. R. Čiegis, Vilnius Gediminas Technical University, Department of Mathematical Modeling, Lithuania, *New trends in parallel algorithms*, October 23.
18. P. Colli, Università di Pavia, Dipartimento di Matematica, Italy, *Long time convergence for a class of phase field models*, May 28.
19. P. Contucci, Università di Bologna, Dipartimento di Matematica, Italy, *Correlation inequalities for spin glasses*, July 9.
20. A. Dalalyan, Université Paris VI, Laboratoire de Probabilités, France, *Exponentially weighted aggregate and estimation under sparsity assumption*, November 26.

21. J. Dudley, Université de Franche-Comté, Laboratoire d'Optique P.M. Duffieux, Besançon, France, *Continual surprises in supercontinuum generation*, February 7.

22. J. Dupačová, Charles University, Department of Probability and Mathematical Statistics, Prague, Czech Republic, *Reflections on risk and dynamics in stochastic programming models*, January 11.

23. Th. Erneux, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, *Analytical studies of quantum dot laser dynamics*, June 12.

24. R. Eymard, Université Paris Est , Département de Mathématiques, Marne-la-Vallée, France, *Approximation of anisotropic heterogeneous diffusion problems on any grids*, February 11.

25. M.H. Farshbaf Shaker, Universität Regensburg, Naturwissenschaftliche Fakultät I – Mathematik, *Über ein nichtlokales viskoses Phasenseparationsproblem*, November 19.

26. M.S. Fofana, Worcester Polytechnic Institute, Mechanical Engineering Department, USA, *Semigroups, generators, spectral decomposition and bifurcation to nonlinear regenerative chatter*, November 21.

27. M. Franke, Universität Jena, Fakultät für Mathematik und Informatik, *Bundle methods for non-convex functions*, January 31.

28. Ch. Geuzaine, University of Liège, Montefiore Institute, Belgium, *Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities, Part I*, December 4.

29. J. Giesselmann, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, *A convergence result for finite volume schemes on Riemannian manifolds*, June 17.

30. R. Glüge, Universität Magdeburg, Institut für Mechanik, *Regularisierung pseudoelastischen Materialverhaltens mit Hilfe einer additiven Viskosität. Teil 1*, May 15.

31. M. Gokieli, Warsaw University, Interdisciplinary Centre for Mathematical and Computational Modelling, Poland, *The reaction-diffusion problem on some special domains*, May 6.

32. Y. Golubev, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, *On statistical testing of true random number generators*, April 22.

33. L.I. Goray, Russian Academy of Sciences, Institute for Analytical Instrumentation, St. Petersburg, *A boundary integral equation method in short-wavelength-to-period diffraction on multilayer 1D gratings and rough mirrors*, October 28.

34. R. Griesse, Technische Universität Chemnitz, Fakultät für Mathematik, *Semismooth Newton methods for portfolio optimization*, September 2.

35. P. Gurevich, Peoples' Friendship University of Russia, Department of Differential Equations and Mathematical Physics, Moscow, *On periodic solutions of thermocontrol problems with hysteresis*, June 3.

36. K. Hackl, Ruhr-Universität Bochum, Lehrstuhl für Allgemeine Mechanik, *Shape-memory alloys, energy-based models for single and polycrystals*, May 14.

37. R. Haller-Dintelmann, Technische Universität Darmstadt, Fachbereich Mathematik, *Maximal parabolic regularity for systems with VMO coefficients*, February 27.

38. H. Hanke, Humboldt-Universität zu Berlin, Institut für Mathematik, *Homogenisierung in der Gradientenplastizität*, December 8.

39. K. Häusler, Ferdinand-Braun-Institut für Höchstfrequenztechnik im Forschungsverbund Berlin e.V., *Experimental investigations of externally wavelength-stabilized broad-area and ridge-waveguide lasers*, November 27.

40. S. Heinz, University of Wyoming, Department of Mathematics, Laramie, USA, *Unified stochastic and deterministic turbulence models*, June 30.

41. Ch. Hennig, University College London, Department of Statistical Science, UK, *How to merge normal mixture components*, November 15.

42. M. Hintermüller, University of Graz, Institute for Mathematics and Scientific Computing, Austria, *Semismooth Newton methods: Theory, numerics and applications*, February 14.

43. M. Hintermüller, Humboldt-Universität zu Berlin, Institut für Mathematik, *PDE-constrained optimization with pointwise control and zero or first order state constraints*, November 25.

44. E. Hög, University of Aarhus, Aarhus School of Business, Finance Research Group, Denmark, *Volatility and realized quadratic variation of differenced returns. A wavelet method approach*, April 30.

45. G.C. Hsiao, University of Delaware, Department of Mathematical Sciences, Newark, USA, *Boundary integral method for an initial-boundary problem in viscous compressible flow*, July 15.

46. S. Ilic, Ruhr-Universität Bochum, Lehrstuhl für Allgemeine Mechanik, *Application of the multi-scale finite element method to a model of composite material*, May 8.

47. O. Iliev, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern, *On modeling and simulations of coupled flows in plain and porous media*, June 24.

48. D. Ioffe, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, *Curie–Weiss model in transverse field and quantum random graphs*, August 6.

49. G. Katriel, Technische Universität Clausthal, Institut für Mathematik, *The explicit spectral theory of discrete one-dimensional Schrödinger operators with finitely supported potentials*, June 18.

50. M. Keller-Ressel, Technische Universität Wien, Institut für Wirtschaftsmathematik, Austria, *Affine processes and applications to stochastic volatility modelling*, January 16.

51. J. Klemelä, University of Oulu, Department of Mathematical Sciences, Finland, *Analysis of the shape of unimodal densities with nonparametric density estimation*, October 29.

52. J. Knobloch, Technische Universität Ilmenau, Institut für Mathematik, *Snaking in reversible systems*, June 24.

53. S.W. Koch, Philipps-Universität Marburg, Fachbereich Physik, and Wissenschaftliches Zentrum für Materialwissenschaften, *VESCEL & Co — Grundlagenphysik in modernen Halbleitermikrolasern*, April 10.

54. L. Korte, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Institut, *The amorphous-crystalline silicon interface — Key for high efficiency silicon heterojunction solar cells*, November 24.

55. M. Kraft, University of Cambridge, Department of Chemical Engineering, UK, *Kinetic models for a more detailed understanding of soot formation and their application to internal combustion engines*, October 29.

56. J. Kreikemeier, Universität Magdeburg, Institut für Mechanik, *Regularisierung pseudoelastischen Materialverhaltens mit Hilfe einer additiven Viskosität. Teil 2*, May 15.

57. A. Kruger, University of Ballarat, School of Information Technology and Mathematical Sciences, Australia, *About extensions of metric regularity*, September 19.

58. K. Krumbiegel, Universität Duisburg-Essen, Fachbereich Mathematik, *On the regularization error of a state constrained Neumann optimal control problem — A virtual control concept*, March 18.

59. J. Kulenkampff, Institut für Interdisziplinäre Isotopenforschung, Leipzig, *Prozesstomographie mit PET zur Ableitung von Transportparametern in Geomaterialien*, June 5.

60. O. Kurbanmuradov, Turkmen State University, Physics and Mathematics Research Center, Ashkhabad, *Stochastic simulation of flows and particles transport in porous media*, November 4.

61. O. Lepski, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, *Universal selection rule in nonparametric estimation*, April 29.

62. M. Lesosky, University of Guelph, Department of Mathematics and Statistics, Canada, *Statistical deconvolution on the Euclidean motion group*, December 3.

63. M. Liero, Humboldt-Universität zu Berlin, Institut für Mathematik, *Derivation of an elastic-plastic plate model by methods of Γ-convergence*, November 10.

64. Y. Liu, Peking University, Department of Mathematics, China, *Long time behaviour of stochastic differential equations*, January 23.

65. D. Löbach, Universität Bonn, Institut für Angewandte Mathematik, *Regularity analysis for hardening problems*, November 26.

66. A. Loose, Humboldt-Universität zu Berlin, Institut für Physik, *Multistability in amplified feedback lasers*, May 8.

67. O. Lopez, Ecole Nationale de la Statistique et de l'Analyse de l'Information, Rennes, France, *Single-index regression models under random censoring*, July 1.

68. Th. Lübben, Universität Bremen, IWT Stiftung Institut für Werkstofftechnik, *Einführung in die Methode des Distortion Engineering*, December 2.

69. M.M. Malamud, Donetsk National University, Department of Mathematics, Ukraine, *Trace formulas and perturbation determinants for a pair of operators*, April 24.

70. ———, *Elliptic, coercive and weakly coercive operators*, December 17.

71. P.M. Mariano, Università degli Studi di Firenze, Dipartimento di Ingegneria Civile e Ambientale, Italy, *Gross scale effects of atomic rearrangements in quasicrystals: Some results and open problems*, February 15.

72. K. Matthies, University of Bath, Department of Mathematical Sciences, UK, *Longtime validity of Boltzmann equations for hard-sphere dynamics*, February 19.

73. P.A. Mayer, Technische Universität Graz, Institut für Optimierung und diskrete Mathematik, Austria, *On the calibration of generalized jump-diffusion models*, April 1.

74. A. Meister, Universität Ulm, Research Training Group 1100 "Modelling, Analysis and Simulation in Economy Mathematics", *Statistical deconvolution problems with Fourier-oscillating error densities*, July 2.

75. H. Michinel, University of Vigo, Faculty of Sciences, Spain, *Generalised nonlinear Schrödinger equations: From matter-wave lasers to quantum liquids*, March 13.

76. G. Milstein, University of Leicester, Department of Mathematics, UK, *Layer methods for Navier–Stokes equations using local probabilistic representations*, October 28.

77. V. Moldoveanu, National Institute of Materials Physics, Laboratory of Low Dimensional Systems, Bucharest, Romania, *Generalized master equation approach to mesoscopic transport*, December 18.

78. G. Müller, Technische Universität München, Zentrum Mathematik, *GARCH and COGARCH: On estimation, convergence and statistical equivalence*, October 22.

79. M. Münzenberg, Universität Göttingen, Physikalisches Institut, *Spinpakete und Spinströme: Wege zur Ultrakurzzeit-Spinelektronik in magnetischen Nanopillarstrukturen*, January 17.

80. J. Naumann, Humboldt-Universität zu Berlin, Institut für Mathematik, *Über die Gleichungen der stationären Bewegung ideal-plastischer Flüssigkeiten*, January 23.

81. G. Nenciu, Romanian Academy, Institute of Mathematics, Bucharest, *Decay laws in perturbation theory of embedded and near threshold eigenvalues*, October 1.

82. Ch.J. Newton, Hewlett Packard Laboratories Bristol, UK, *Modelling for paper-like displays*, May 26.

83. S. O'Brien, Tyndall National Institute, Cork, Ireland, *Discrete mode Fabry–Perot lasers: Design approach and non-linear dynamical properties*, December 18.

84. S. Ogawa, Ritsumeikan University, Department of Mathematical Sciences, Kusatsu, Japan, *On the volatility estimation in the presence of microstructure noise*, November 16.

85. O. Omel'chenko, Humboldt-Universität zu Berlin, Institut für Mathematik, *Chimera states: The natural link between coherence and incoherence*, July 8.

86. H.-Ch. Öttinger, Eidgenössische Technische Hochschule Zürich, Institut für Polymere, Switzerland, *Hydrodynamics, Thermodynamics, and Mathematics*, June 30.

87. J. Outrata, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, *On a class of optimal control problems within mathematical programs with equilibrium constraints*, December 8.

88. L. Panizzi, Scuola Normale Superiore, Pisa, Italy, *A uniqueness and stability result for a quasilinear parabolic system*, June 10.

89. V. Panov, StatSoft Russia, Moscow, *Quantum bit commitment*, June 17.

90. L. Paoli, Université de Saint-Etienne, Laboratoire de Mathématiques, France, *Existence and approximation for a 3D model of thermally induced phase transformations in shape-memory alloys*, January 30.

91. V. Patilea, Institut National des Sciences Appliquées (INSA) de Rennes, Centre des Mathématiques, France, *Bandwidth-robust inference with conditional moment restrictions*, May 7.

92. A. Pimenov, University College Cork, School of Mathematical Sciences, Ireland, *Numerical study of nonlinear dynamical regimes in a passively mode-locked semiconductor laser*, May 22.

93. M. Podolskij, University of Aarhus, Institute for Economy, Denmark, *Inference for quadratic variation of semimartingales in the presence of noise*, April 16.

94. E.R. Racec, Brandenburgische Technische Universität Cottbus, Lehrstuhl für Theoretische Physik I, *Interacting electron systems in external fields. Part 1: Field quantization method*, December 3.

95. ———, *Interacting electron systems in external fields. Part 2: Response functions*, December 18.

96. B. Rech, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Institut, *Solarzellen an dünnen Siliziumschichten — Stand der Technik und Herausforderungen für die Zukunft*, November 24.

97. L. Recke, Humboldt-Universität zu Berlin, Institut für Mathematik, *Differentiability and non-differentiability of Nemycki operators and related problems in mathematical modeling*, February 7.

98. ———, *Smoothness of solutions and smoothness of the data-to-solution map for 2D Signorini problems*, November 26.

99. T. Rees, Oxford University, Computing Laboratory, UK, *Preconditioning iterative methods for PDE constrained optimization*, April 22.

100. J.-F. Remacle, Université Catholique de Louvain, Center for Systems Engineering and Applied Mechanics, Louvaine-la-Neuve, Belgium, *Gmsh: A three-dimensional finite element mesh generator with built-in pre- and post-processing facilities, Part II*, December 4.

101. H. Riechert, Paul-Drude-Institut für Festkörperelektronik im Forschungsverbund Berlin e.V., *Wissenschaftliche Schwerpunkte am Paul-Drude-Institut*, May 26.

102. W. Ring, Karl-Franzens-Universität Graz, Institut für Mathematik, Austria, *Geodesics and parallel transport in implicit shape space*, July 22.

103. E. Rocca, Università degli Studi di Milano, Dipartimento di Matematica "F. Enriques", Italy, *Degenerating PDEs for phase transitions in thermoviscoelastic materials*, November 4.

104. E. Rohan, University of West Bohemia, Faculty of Applied Sciences, Plzen, Czech Republic, *Homogenization of acoustic transmission through a periodically perforated layer*, December 3.

105. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, *Mathematical techniques for rate-independent processes*, February 6.

106. D. Rudolf, Friedrich-Schiller-Universität Jena, Mathematisches Institut, *Explicit error bounds for lazy reversible Markov chain Monte Carlo*, May 27.

107. U. Sack, Freie Universität Berlin, Institut für Mathematik, *Numerical simulation of binary alloys*, November 17.

108. A.-M. Sändig, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, *Griffith's fracture criterion in piezoelectric ceramics*, January 9.

109. A. Scheel, University of Minnesota, School of Mathematics, Minneapolis, USA, *How robust are Liesegang patterns*, May 6.

110. M. Schieck, Technische Universität Chemnitz, Fakultät für Mathematik, *Conditional stability for general linear regularization methods*, April 1.

111. A. Schiela, Konrad-Zuse-Zentrum für Informationstechnik Berlin, *Optimalitätsbedingungen für zustandsbeschränkte Optimalsteuerungsprobleme bei unstetigen Zuständen*, May 27.

112. S. Schikora, Humboldt-Universität zu Berlin, Institut für Physik, *Global properties of optical chaos control*, May 15.

113. F. Schilder, University of Surrey, Department of Mathematics, Guildford, UK, *Computational bifurcation analysis of Hamiltonian relative periodic orbits*, December 9.

114. G.R. Sell, University of Minnesota, School of Mathematics, Minneapolis, USA, *On the theory and applications of the longtime dynamics of 3-dimensional fluid flows on thin domains*, December 2.

115. V. Seremet, Agrarian State University, Chisinau, Republic of Moldova, *Derivation of Green's formulae for elasticity problems*, November 4.

116. J. Sokołowski, Université de Nancy I, Laboratoire de Mathématiques, Vandœuvre-lès-Nancy, France, *Rigid inclusions and cracks: Modeling and shape sensitivity analysis*, October 21.

117. V.A. Solonnikov, Steklov Institute of Mathematics, Petersburg Department, Laboratory of Mathematical Physics, Russia, *On some evolution-free boundary problems for the Navier–Stokes equations*, April 16.

118. J.-U. Sommer, Leibniz-Institut für Polymerforschung Dresden, *Eine kurze Geschichte der Polymerphysik: Von Naturkautschuk zu Nanostrukturen*, December 15.

119. Ch. Sparber, University of Cambridge, Department of Applied Mathematics and Theoretical Physics, UK, *On the Gross–Pitaevskii equation for trapped dipolar quantum gases*, July 2.

120. K. Staliunas, Universitat Politecnica de Catalunya, Departament de Fisica i Enginyeria Nuclear, Barcelona, Spain, *Rocking of lasers: Rocking in time, but now also in space*, December 8.

121. R. Stangl, Helmholtz-Zentrum für Materialien und Energie, Bereich Silizium-Photovoltaik, Berlin, *Rückseitenkontaktierte a-Si:H/c-Si Heterosolarzellen: Prozessierung/Charakterisierung/Simulation*, November 5.

122. G. Steinmeyer, Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie im Forschungsverbund Berlin e.V., *Pulse self-compression in filaments*, November 6.

123. A. Teplinsky, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, *Smooth conjugacy of circle diffeomorphisms with singularities*, October 21.

124. M. Thomas, Humboldt-Universität zu Berlin, Institut für Mathematik, *Existence of an energetic solution for a rate-independent damage process*, July 3.

125. V. Tkachenko, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, *Slowly oscillating wave solutions of a single-species reaction-diffusion equation with delay*, October 14.

126. M. Tlidi, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, *Localized beating between dynamically generated frequencies*, November 20.

127. A. Torcini, Consiglio Nazionale delle Ricerche, Istituto dei Sistemi Complessi, Florence, Italy, *Chaotic synchronization in spatially extended systems*, April 22.

128. K. Trivisa, University of Maryland, Department of Mathematics, College Park, USA, *From the dynamics of gaseous stars to the incompressible Euler equations*, July 9.

129. V.Z. Tronciu, Technical University of Moldova, Department of Physics, Chisinau, Moldova, *Chaos based communication using multi-section semiconductor laser*, April 24.

130. D. Turaev, Imperial College London, Department of Mathematics, UK, *The Lorenz attractor does exist*, August 26.

131. N. Vayatis, Ecole Normale Supérieure de Cachan, Centre de Mathématiques et de Leurs Applications, France, *ROC curve optimization*, June 18.

132. E. Verbree, Delft University of Technology, OTB Institute for Housing, Urban and Mobility Studies, The Netherlands, *GIS-Technology: Spatial data handling of polyhedra through constrained Delaunay tetrahedralization*, October 16.

133. E.A. Viktorov, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, *Recovery dynamics in quantum dot structures*, December 4.

134. U. von Luxburg, Max-Planck-Institut für Biologische Kybernetik, Tübingen, *Consistent minimization of clustering objective functions*, May 20.

135. H. Wenzel, Ferdinand-Braun-Institut für Höchstfrequenztechnik im Forschungsverbund Berlin e.V., *Thermal lensing in high-power ridge-waveguide lasers*, January 31.

136. J. Wölk, Universität Köln, Institut für Physikalische Chemie, *Homogene Keimbildung: Experiment vs. Theorie*, April 22.

137. H. Wu, Fudan University, School of Mathematical Sciences, Shanghai, China, *Convergence to equilibrium for nonlinear evolution equations*, October 29.

138. M. Yamamoto, University of Tokyo, Department of Mathematical Sciences, Japan, *Inverse problems in mechanics related to elasticity*, April 29.

139. ———, *Reconstruction of the coefficients in the Stefan–Boltzmann boundary condition for the heat process*, September 16.

140. Q. Yao, London School of Economics, Department of Statistics, UK, *Modelling high-dimensional daily volatilities based on high-frequency data*, July 8.

141. I. Yousept, Technische Universität Berlin, Institut für Mathematik, *State constrained optimal control of semilinear elliptic equations with nonlocal radiation interface conditions*, January 24.

142. Ch. Zanini, University of Udine, Department of Mathematics and Computer Science, Italy, *Periodic solutions and complex dynamics for a differential equation arising in the study of a nerve fiber model*, June 4.

143. O. Zindy, Université Paris VI, Laboratoire de Probabilités et Modèles Aléatoires, France, *Random walks in random environment: Localization studies*, April 28.

A.14 Software

adimpro (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: tabelow@wias-berlin.de)

adimpro is a contributed package within the R-Project for Statistical Computing that contains tools for image processing, including structural adaptive smoothing digital color images. The package is available from the Comprehensive R Archive Network (http://cran.r-project.org).

AWS (contact: J. Polzehl, phone: +49 30/20372-481, e-mail: polzehl@wias-berlin.de)

AWS is a contributed package within the R-Project for Statistical Computing that contains a reference implementation of the adaptive weights smoothing algorithms for local constant likelihood and local polynomial regression models. Binaries for several operating systems are available from the Comprehensive R Archive Network (http://cran.r-project.org).

AWS for AMIRA (TM) (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: tabelow@wias-berlin.de)

This plugin implements a structural adaptive smoothing procedure for two- and three-dimensional medical images in the visualization software AMIRA (TM). It is available in the Zuse Institute Berlin's version of the software for research purposes (http://amira.zib.de/).

BOP (contact: J. Borchardt, phone: +49 30/20372-485, e-mail: borchardt@wias-berlin.de)

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, but can also be run efficiently on different single processor machines, as well as under LINUX or Windows XP. 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, e-mail: mucha@wias-berlin.de)

The statistical software ClusCorr98® performs exploratory data analysis with the focus on cluster analysis, classification, and multivariate visualization. A highlight is pairwise data clustering for finding groups in data. Another highlight is the automatic validation technique of cluster analysis results performed by a general built-in validation tool that is based on resampling techniques. It 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 well-known measures of correspondence between partitions. Second, the stability of each individual cluster is assessed based on measures of similarity between sets. It 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® runs in the host application Excel 2007. Hence it makes use of the new "Big Grid" spreadsheets.

Further information: http://www.wias-berlin.de/software/ClusCorr98

DiPoG (contact: A. Rathsfeld, phone: +49 30/20372-457, e-mail: rathsfeld@wias-berlin.de)

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.

dti (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: tabelow@wias-berlin.de)

dti is a contributed package within the R-Project for Statistical Computing. The package contains tools for the analysis of diffusion-weighted magnetic resonance imaging data (DWI) in the context of the diffusion tensor (DTI) model. It can be used to read DWI data, to estimate the diffusion tensor, for adaptive smoothing of DWIs, and for two- and three-dimensional visualization of the results. The package is available from the Comprehensive R Archive Network (http://cran.r-project.org).

EDR (contact: J. Polzehl, phone: +49 30/20372-481, e-mail: polzehl@wias-berlin.de)

EDR is a contributed package within the R-Project for Statistical Computing that contains tools for the efficient estimation of dimension reduction spaces in multi-index models. The package is available from the Comprehensive R Archive Network (http://cran.r-project.org).

gltools (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: fuhrmann@wias-berlin.de)

gltools is a library for the visualization of finite volume and finite element computations on unstructured triangular and tetrahedral meshes. Unlike many other packages, it has been designed in such a way that it can be integrated into the numerical solution process. Therefore, the software package can be used not only for the support of pre- and postprocessing, but also for debugging during the development of numerical algorithms. In particular, gltools can be used as an integral part of the toolbox pdelib. Using the OpenGL API, it provides efficient visualization of time-dependent scalar and vector data on one-, two-, and three-dimensional simplicial grids. The graphical user interface is based on the FLTK toolkit.

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

fmri (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: tabelow@wias-berlin.de)

fmri is a contributed package within the R-Project for Statistical Computing that contains tools to analyze fMRI data with structure adaptive smoothing procedures. Binaries for several operating systems are available from the Comprehensive R Archive Network (http://cran.r-project.org).

LDSL-tool (contact: M. Radziunas, phone: +49 30/20372-441, e-mail: radziunas@wias-berlin.de)

`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 and different coupled laser devices. This software is used to investigate and to design laser devices that exhibit various nonlinear effects such as self-pulsations, chaos, hysteresis, mode switching, excitability, mutual synchronization and frequency entrainment by an external modulated optical or electrical signal.

`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, e-mail: fuhrmann@wias-berlin.de)

`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-3dReduce (contact: I. Bremer, phone: +49 30/20372-315, e-mail: bremer@wias-berlin.de)

Based on SGI's OpenGL Performer and COG, this is a software for optimizing the visualization performance of three-dimensional objects in a virtual reality environment. It reduces the number of surface vertices and triangles with or without changing the visible geometry. Automatic level-of-detail generation is included. Many three-dimensional formats are supported through Performer loader plugins, especially VRML, Open Inventor, and Realax. The package is distributed as part of Rücker Factory Invision by Rücker EKS GmbH (holger.haemmerle@ruecker.de) under the name `rfreduce`.

A web interface for a demo version is available on request at
`http://www.wias-berlin.de/~bremer/cgi/reduce/reduce`.

WIAS-HiTNIHS (contact: O. Klein, phone: +49 30/20372-533, e-mail: klein@wias-berlin.de)

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 induction or resistance heating. 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. It is also possible to use `WIAS-HiTNIHS` just to compute axisymmetric magnetic scalar potentials, the resulting magnetic fields and/or the resulting heat sources. In particular, one can compute so-called *traveling magnetic fields* and resulting Lorentz forces acting on conducting liquids.

The simulator is designed to deal with complicated axisymmetric setups having a polygonal two-dimensional 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 is further developed within the project *Numerical simulation and control of sublimation growth of semiconductor bulk single crystals*, supported by the DFG (since 2002), http://www.wias-berlin.de/publications/annual_reports/2004/node79.html.

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

WIAS-MatConE (contact: O. Klein, phone: +49 30/20372-533, e-mail: klein@wias-berlin.de)

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: W. Weiss, phone: +49 30/20372-478, e-mail: weiss@wias-berlin.de)

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 automatic adaptive grid based on error estimation 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, e-mail: nuernberg@wias-berlin.de)

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, lasers, and solar cells.

The semiconductor device simulation package WIAS–TeSCA operates in a Linux environment on desktop computers.

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

WIAS-QW (contact: Th. Koprucki, phone: +49 30/20372-508, e-mail: koprucki@wias-berlin.de)

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.