W I A S

Weierstrass Institute for Applied Analysis and Stochastics

Leibniz Gemeinschaft

Forschungsverbund Berlin e.V.

Intelligent solutions for complex problems

Annual Research Report 2007

Cover figure: Numerical simulation of the formation of spatiotemporal optical solitons mediated by a “neck”-type modulational instability in an array of coupled waveguides

Edited by Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
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ISSN 1437-7489
Berlin 2007

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Prof. Dr. Jürgen Sprekels, Director

The Weierstrass Institute for Applied Analysis and Stochastics (WIAS, member of the Leibniz Association) presents its Annual Report 2007. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2007. Following a more general introduction in part one, in its second part five 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 2007 was marked by taking up the 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
- Stochastics in science and economics
- Flow and transport processes in continua
- 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. For the first time, the total grants aquired in 2007 crossed the “magical border” of two million euros. More than thirty additional co-workers could be financed from these grants.

In addition to this, WIAS was in 2007 for the first time successful in the Excellence Competition of the Leibniz Association: Dr. Jürgen Fuhrmann will head from 2008 to 2010 a network on “Coupled flow processes in energy and environmental research”, which includes groups from several research institutes and universities. The cooperation partners WIAS, Free University of Berlin, University of Erlangen-Nürnberg, and Potsdam Institute for Climate Impact Research got six scientific positions, two of which are located at WIAS.

The extraordinary increase in the number of refereed journal publications achieved in 2006 was in 2007 followed by a “normal” ouput, to which four excellent monographs added, which were authored or edited by WIAS members and which appeared in renowned scientific series of top-selling publishing companies. Each one of these monographs marks a milestone and culmination point of long-standing research at WIAS, and is visible evidence for the scientific excellence of its collaborators.

As another highlight of 2007, the Director of WIAS was invited to deliver an address to the “Science and Technology in Society (STS) Forum” in Kyoto, Japan. In this high-ranking event, he was one of very few mathematicians who served as speakers.

The high rank of WIAS in the mathematical community is also witnessed by the fact that the year-long success story of "Transfer of knowledge via brains" through the institute's members continued also in 2007: Dr. Denis Belomestny was offered a Junior Professorship at the Humboldt University of Berlin, which he declined. Since the institute's foundation in 1992, a total of 34 calls (including 16 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. Also remarkable is the fact that since 2003 no less than three female members of WIAS have been called to university professorships.

Four 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. Alexander Mielke served as co-organizer of a conference at the Mathematisches Forschungsinstitut Oberwolfach (MFO). Also the guest program of WIAS was intensified in 2007 by hosting the group of winners of the Weierstrass Postdoctoral Fellowships (see page 123).

In addition to these "global" activities, WIAS has on the "local" scale intensified its well-established cooperation with the other mathematical institutions in Berlin, with the main attention directed toward the three Berlin universities. This is witnessed by the fact that as of today five leading members of WIAS, including the director and his two deputies, hold special chairs funded by WIAS at the Berlin universities. Another such appointment is under way, and we are hoping that by the end of 2008 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 2007 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 a member of MATHEON's Executive Board, both his deputies are "Scientists in Charge" of mathematical fields in the center, and members of WIAS participate in the management of 18 of its subprojects. In turn, in 2007 up to 16 scientific collaborators and several student assistants employed at WIAS were funded by MATHEON.

Another big success story for the mathematical community of Berlin was the successful start of 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, the second Deputy Director of WIAS, is 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 participated in the successful application for the DFG Collaborative Research Center "Semiconductor Nanophotonics: Materials, Models, Devices" (SFB 787) at the Technical University of Berlin.

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 March 2008

J. Sprekels

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1 WIAS in 2007

- 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.

1.2 Structure and Scientific Organization

1.2.1 Structure

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

RG 1. Partial Differential Equations

RG 2. Laser Dynamics

RG 3. Numerical Mathematics and Scientific Computing

RG 4. Nonlinear Optimization and Inverse Problems

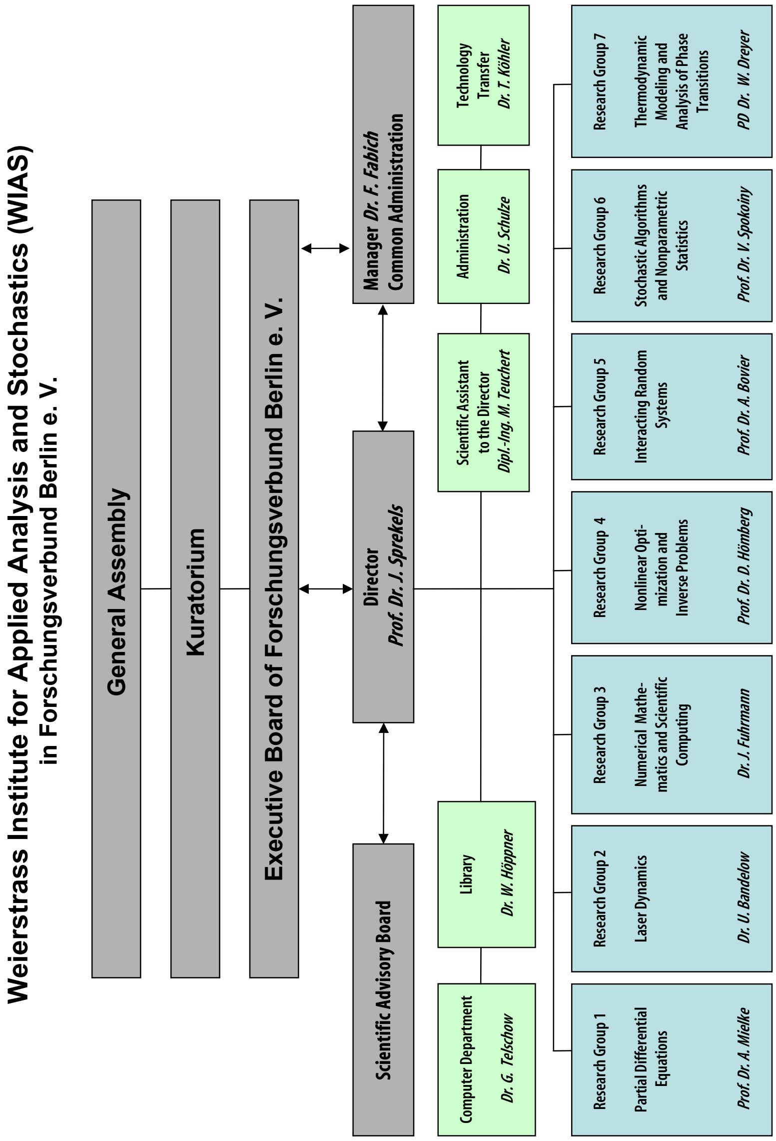
RG 5. Interacting Random Systems

RG 6. Stochastic Algorithms and Nonparametric Statistics

RG 7. Thermodynamic Modeling and Analysis of Phase Transitions

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

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



1.2.2 Main Fields of Research

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

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

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

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

1.2.3 Contributions of the Research Groups of WIAS

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

The following table gives an overview to which main fields the research groups have contributed in 2007 in the interdisciplinary solution process described above.

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

In the following, we list special research topics that have been addressed in 2007 within the general framework of the main fields. The research groups that have contributed to the respective studies are indicated in brackets.

1. Nano- and optoelectronics

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

2. Optimization and control of technological processes

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

3. Phase transitions and multifunctional materials

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

4. Stochastics in science and economics

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

5. Flow and transport processes in continua

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

6. Numerical methods of analysis and stochastics

- Numerical solution of partial differential equations (finite volume and finite element methods, preconditioners, grid generation, error estimators, and adaptivity; in all research groups, especially in RG 3)
- Numerics of inverse problems (integral equations, regularization techniques; in RG 1, RG 4, and RG 6)
- Nonlinear optimization techniques (in RG 4)
- Stochastic numerics (Monte Carlo methods, kinetic equations, coagulation dynamics, particle systems; in RG 5, RG 6, and RG 7)
- Development of WIAS software packages (see page 134)

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 2007, having raised a total of 2.044 million euros, from which additional 30 (+ 4 outside WIAS) researchers (Dec. 31, 2007) have been financed. Particularly important is the fact that the funds raised in industrial collaborations could be increased to 356,000 euros. In total, 23.19 per cent of the total budget of WIAS in 2007 and 35.71 per cent of its scientific staff originated from grants. In the following, some projects of particular interest and importance will be highlighted, without going into too much detail[2].

1.3.1 DFG Research Center MATHEON

The highlight of cooperation with the mathematical institutions in Berlin has been the joint operation of the DFG Research Center MATHEON "Mathematics for key technologies". 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. WIAS dedicates considerable financial and personal resources to the Center: its director is a member of MATHEON's Executive Board, both his deputies are "Scientists in Charge"

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

of mathematical fields in the Center, and members of WIAS participate in the management of 18 of its subprojects. In turn, in 2007 up to 16 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 contribute to the operations of the BMS.

1.3.3 International Research Training Group *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, the second Deputy Director of WIAS.

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

In the Research Training Group GRK 1128 at Humboldt-Universität zu Berlin, which started operations in April 2005 (first funding period: until September 2009), a number of WIAS members are active as principal investigators and associate members; Prof. D. Hömberg (RG 4) has been its Deputy Coordinator until March 2007. WIAS members are presently supervising the theses of seven graduates.

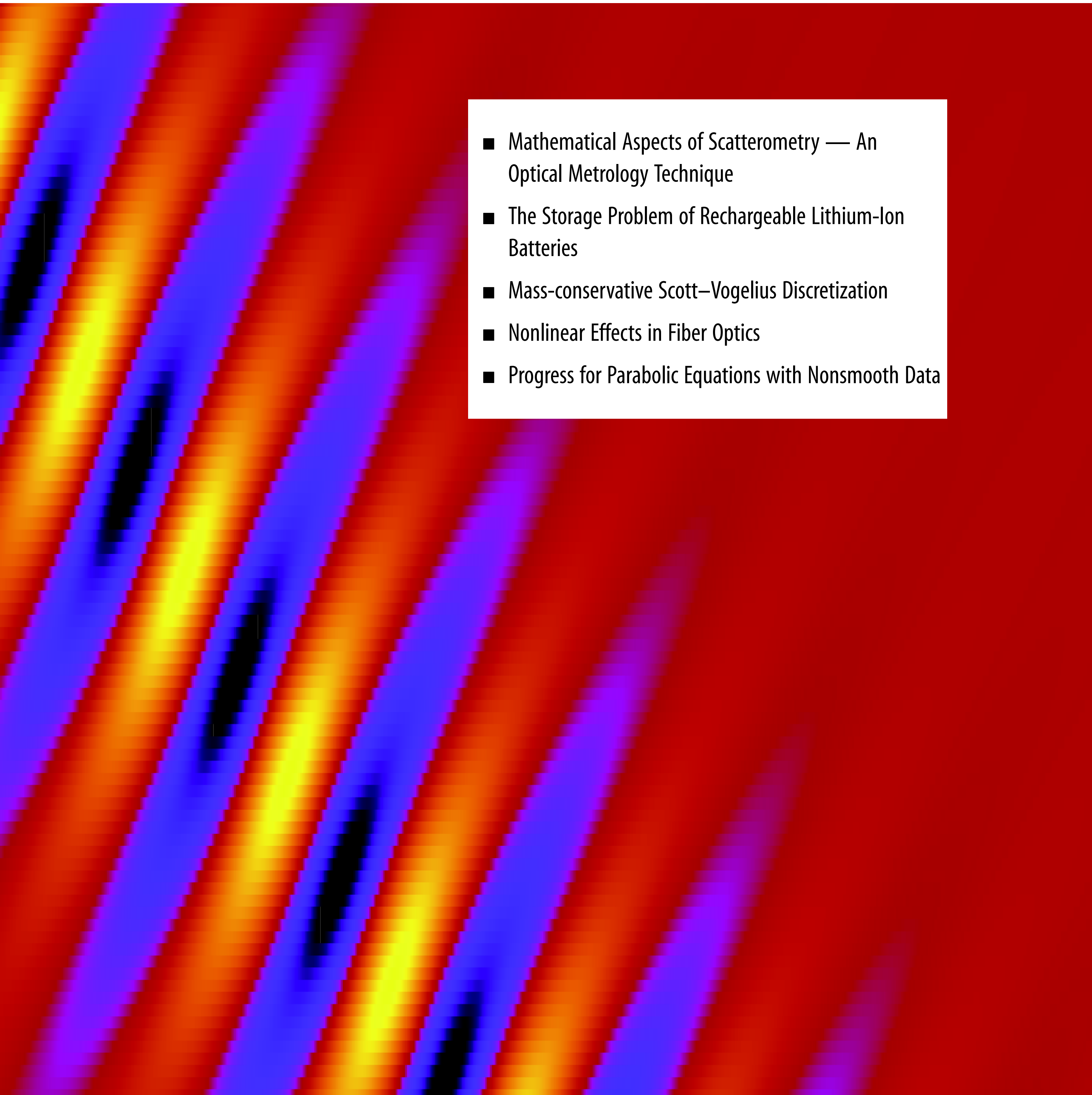
1.3.5 KRIST*MAG*

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

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

This research project, which started operations in 2005 and will run until June 2008, is 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 is part of an interdisciplinary joint project for the experimental investigation, modeling, and numerical simulation of direct methanol micro fuel cells, which is coordinated by the acting head of RG 3, Dr. J. Fuhrmann.

2 Scientific Highlights



- Mathematical Aspects of Scatterometry — An Optical Metrology Technique
- The Storage Problem of Rechargeable Lithium-Ion Batteries
- Mass-conservative Scott–Vogelius Discretization
- Nonlinear Effects in Fiber Optics
- Progress for Parabolic Equations with Nonsmooth Data

2.1 Mathematical Aspects of Scatterometry — An Optical Metrology Technique

Hermann Groß (Department 8.4 of Mathematical Modelling and Data Analysis, Physikalisch-Technische Bundesanstalt (PTB)) and Andreas Rathsfeld

Scatterometry and alternative methods of measurement

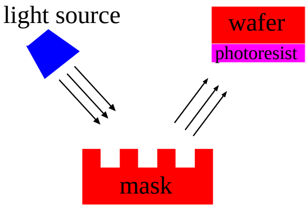


Fig. 1: *Illumination of wafer with light scattered by mask*

The breathtaking development of nanotechnology requires to design and control components with ever smaller details. In particular, the fabrication of up-to-date computer chips and storage devices by lithographic manufacturing processes is impossible without new accurate measurement techniques coping with the tiny details of masks and wafers. A promising approach for the chip production of the next generation is extreme ultraviolet (EUV) lithography. Recall that, simply speaking, lithography is like old-fashioned photography. The EUV light, scattered by a mask, illuminates a photoresist layer on the wafer, thus forming an image of the mask structure (see Figure 1). Similarly to developing films in photography, baking and etching processes fix the mask structure on the wafer. In other words, a new chip with the given mask structure is fabricated. The lateral dimensions of a typical structure in EUV lithography may be in the size of about twenty nanometers. The vertical heights of the various layers forming such structures, however, are up to one nanometer.

The usual methods of mask measurements are scanning electron microscopy (SEM) or atomic force microscopy (AFM). In SEM, the signals of backscattered electrons or secondary electrons from a surface scan are used to determine the profile parameters. In AFM, the deflection of the sharp tip at the end of a microscale cantilever is used to scan the specimen surface. Unfortunately, these methods do not necessarily yield the same results. Furthermore, both have their specific limitations. Scatterometry is an independent and alternative technique for the characterization of mask profiles. In scatterometry, the sample is illuminated by a light with a wavelength comparable with or even larger than the details to be determined. Of course, instead of a nice image, a picture of a complicated scattered wave pattern is measured. The true geometry must be reconstructed by solving an inverse problem for the electromagnetic wave equations (time-harmonic Maxwell system). More precisely, using a numerical algorithm, a geometry with such details is to be sought for which the diffraction pattern of the numerical simulation coincides with the measured pattern. If this inverse problem is solved, then scatterometry provides a new indirect (non-imaging) and nondestructive measurement method.

Unfortunately, the inverse problem is what mathematicians call a *severely ill-posed problem*. In other words, small measurement perturbations in the scattering pattern can amount to huge deviations for the reconstructed geometry. Therefore, a reconstruction of a general geometry is impossible. Physicists call this well-known fact the *diffraction limit*: measurement methods based on electromagnetic waves provide details only up to the size of the wavelength and not smaller. On the other hand, scatterometry does not have to reconstruct a completely unknown geometry. Usually, the main features of the structure are already known, and only a few numbers (parameters) are missing. For example, in case of a certain manufacturing process, we may assume that the geometric detail is an elongated line (bridge) with trapezoidal cross section. The unknown parameters are, for example, the height of the bridge, the sidewall angles (SWA), and the upper or lower horizontal width of the trapezoid, which are called *upper and lower critical dimensions (CD)*. This inverse problem of parameter identification is well posed, and an accurate approximation of the interesting geometric parameters by accurate numerical algorithms should be possible.

Measurement setups and simulation

The first important benchmark test for the lithographic production is to generate line-space structures and to check the accuracy of their dimensions. More precisely, on a sample with a plane surface, a group of parallel lines (bridges) is placed. All these bridges have the same trapezoidal cross section in the plane perpendicular to the line direction (groove direction). Due to equal spaces (distances of bridges in surface direction perpendicular to the groove direction), the line-space structure forms a so-called *grating*, which is constant in the groove direction and periodic in the surface direction perpendicular to the grooves. We shall restrict our further considerations to the measurement of gratings.

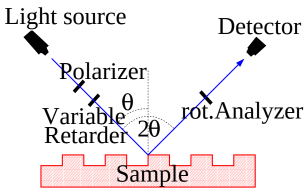


Fig. 2: *Setup of scatterometric measurement*

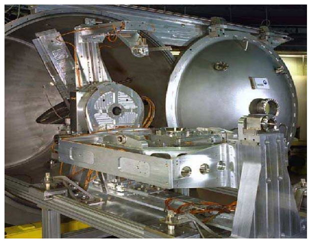


Fig. 3: *EUV reflectometer (PTB WG 7.12)*

In scatterometry (see Figure 2), a polarized light ray illuminates the sample for measurement under various angles of incidence Θ and with different wavelengths. The light is scattered by the sample, and the outgoing wave is measured in various directions of radiation. The PTB has the measuring apparatuses working in the visible, the deep ultraviolet, and the EUV light ranges (see Figure 3 for EUV scatterometry). Typically, in case of gratings, the direction of the inspecting light ray is chosen to be inside the cross-section plane perpendicular to the groove direction. Then the resulting scattered wave directions are located in the same plane. Due to the periodicity of the grating structure, the outgoing light propagates only into a finite number of directions. Now, the scatterometer measures the so-called *efficiencies*, i.e., the portion of energy conveyed to these discrete outgoing rays. Additionally, the phase differences of the outgoing light rays corresponding to differently polarized inspecting waves can be determined. Though the directions of the scattered waves are independent of the shape of the sample, the efficiencies and phase differences strongly depend on the grating geometry. Consequently, the mathematical part in scatterometry is to determine (reconstruct) the geometric parameters of the grating structure from the measured efficiencies and/or phase differences.

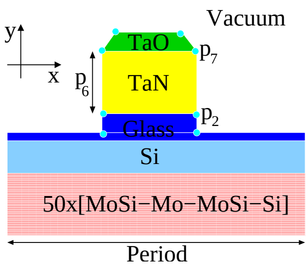


Fig. 4: *EUV line-space structure*

Figure 4 shows the cross section over one period (840 nm) of a typical line-space structure for EUV lithography. The line is a symmetric bridge made of three layers of different materials. The bottom CD is about 140 nm, and a multilayer system beneath the line-space structure enables the reflection of the EUV waves. Interesting geometric parameters are, e.g., the height $p_6 \approx 55\,nm$ of the tantalum layer and the relative x-coordinates $p_2 \approx 490/840$ and $p_7 \approx 490/840$ of the right corners of the tantalum layer.

To analyze the relation between the parameters $p_j,\ j = 1, \dots, J$, describing the geometric shape of the grating structure and the resulting efficiencies $E_m = E_m(p_1, \dots, p_J),\ m = 1, \dots, M$, of the scattered wave modes, the light diffraction has to be simulated. Clearly, the electromagnetic waves can be described by the time-harmonic Maxwell system. In the case of grating structures, this system reduces to a single Helmholtz equation (cf. [6])

$$\Delta u(x) + k^2 u(x) = 0, \quad x \in \mathbb{R}^2,$$

where k is the wave number of the light, and u is the transversal field component oscillating in the groove direction. If the electric field of the incoming wave is oscillating only in the groove direction (TE polarization), then u is the transversal component of the electric field. For incoming light with the magnetic field vector oscillating only in the groove direction (TM polarization), u is the transversal magnetic component. All the other field components can be derived from u. In particular, the efficiencies E_m and the phase differences can be computed by well-known integral formulas including u. In order to determine the field component u itself, we have to find a solution to:

- the Helmholtz equation in each domain with materials of the same refractive index
- transmission conditions on the interfaces between different domains
- special boundary conditions on the lateral boundaries of one period of the cross-section domain
- a special radiation condition for the behavior at infinity

For the numerical solution of this boundary value problem, several numerical algorithms are available (cf., e.g., [6,5]). We have developed a program package called DiPoG, which is based on a generalized finite element method (FEM). Besides the computation of efficiencies for grating structures with a given geometry, the FEM technique enables the determination of the first-order derivatives of the efficiencies E_m with respect to the geometric parameters p_j; cf. [1].

Reconstructing geometric details from measured wave data

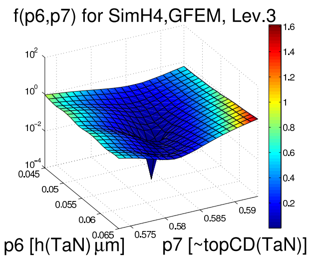


Fig. 5: *2D section of least-squares functional* Φ

In general, it is not clear if the geometric data can really be reconstructed from the measurements. There exist sophisticated mathematical theorems claiming that the knowledge of the complete reflected field for a single or a few incident plane-wave illuminations determines the geometry of the grating uniquely. However, to decide whether reconstruction is possible for a finite number of measurement values and a finite number of reconstruction parameters is much more difficult. Nevertheless, we should be optimistic if the number of measurements is larger than that of the parameters to be reconstructed. Only in exceptional cases reconstruction may not be realistic. For instance, the simultaneous determination of the heights of the tantalum and the tantalum oxide layer for the structure in Figure 4 is difficult since the optical properties (refractive indices) of both materials are similar.

Now suppose the measured efficiency data is denoted by E_m^{meas}, $m = 1, \ldots, M$. Then, reconstructing the geometry means to find the solution p_j^{sol}, $j = 1, \ldots, J$, to the nonlinear system $E(p_1, \ldots, p_J) = E_m^{\text{meas}}$, $m = 1, \ldots, M$. Equivalently, a vector (p_j^{sol}) has to be found at which the following nonlinear and nonconvex least-squares functional (see Figure 5) attains its minimum:

$$\Phi(p_1, \ldots, p_J) := \sum_{m=1}^{M} w_m \left| E_m(p_1, \ldots, p_J) - E_m^{\text{meas}} \right|^2 .$$

Here, the w_m are suitably chosen weight factors, which should be adjusted to the measurement uncertainties of the E_m. For instance, w_m could be chosen as the squared reciprocal uncertainty value. We seek a solution vector of our optimization problem in the class of vectors (p_j) satisfying the constraints $p_j^{\min} \leq p_j \leq p_j^{\max}$, $j = 1, \ldots, J$. Approximations for (p_j) can be computed using standard optimization routines; cf. [2]. We have obtained nice results applying the interior point method and the Gauss–Newton algorithm implemented in DiPoG; cf. [3, 4]. Note that these schemes are based on the gradient computation by FEM; cf. [1]. Figures 6 and 7 show the initial and final solution of a Gauss–Newton iteration for the reconstruction of p_2, p_6, and p_7.

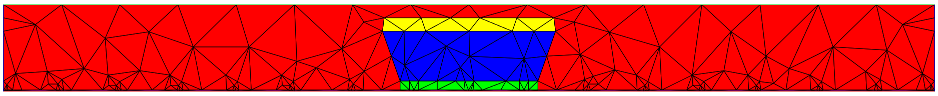


***Fig. 6:** Initial solution of Gauss–Newton iteration*

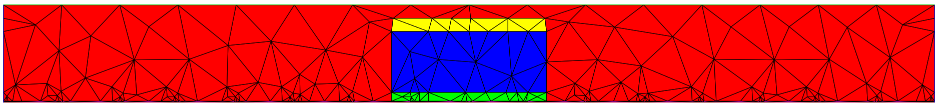


***Fig. 7:** Final solution of Gauss–Newton iteration*

Unfortunately, the mentioned optimization algorithms converge only to vectors with local minima. In other words, the numerical approximation (p_j^{sol}) fulfills $\Phi(p_1^{\mathrm{sol}}, \ldots, p_J^{\mathrm{sol}}) \leq \Phi(p_1, \ldots, p_J)$ for all vectors (p_j) close to (p_j^{sol}) only. To get the true solution (global minimum solution), a good starting guess is needed, or the numerical algorithm must be started from several initial solutions, and the local solution with the smallest functional value is declared the global solution. Alternatively, one can employ global optimization schemes like simulated annealing or genetic algorithms. These schemes, however, seem to be extremely time-consuming.

Optimal setups for the reconstruction

So far, the set of measured data can be arbitrary. Of course, the number of data should be larger than or equal to the number J of unknown parameters. From a "statistical" point of view, one would expect that as much data as possible should be measured. The more information one has, the more accurate the reconstruction result is. On the other hand, using more data means an increased number of measurements and, probably, a huge amount of work for the numerical conversion of measurement data in geometric parameters. If not the whole possible data is used, then the question arises as to which entities should be measured. For which set of measurements is the correspondence of measurements (E_m) to parameters (p_j) the most suitable? After the set of all possible measurements is fixed, it is the duty of the mathematicians to find out which subset of measurements is the most convenient. Indeed, the mapping $(p_j) \mapsto (E_m = E_m(p_1, \ldots, p_J))$ can be analyzed by numerical simulation. We introduce the Jacobian matrix of the mapping $\mathcal{J} := (\partial E_m / \partial p_j)_{m,j}$, with m running through the index set of an appropriate subset of measurement data, and accept the condition number

$$\kappa := \frac{\max_{j=1,\ldots,J} |\mathrm{eigenvalue}_j(\mathcal{J}^\top \mathcal{J})|}{\min_{j=1,\ldots,J} |\mathrm{eigenvalue}_j(\mathcal{J}^\top \mathcal{J})|}$$

as a quality measure of the mapping $(p_j) \mapsto (E_m)$. The smaller κ, the better the mapping $(p_j) \mapsto (E_m)$, and the better the choice of measured data included in the mapping. Indeed, minimizing κ consists in minimizing the maximal eigenvalue of $\mathcal{J}^\top \mathcal{J}$ and maximizing the minimal eigenvalue

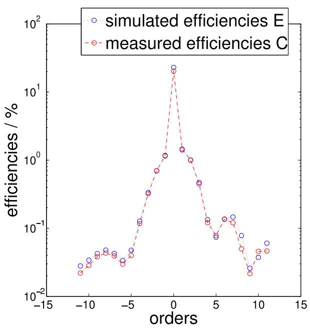


Fig. 8: *Efficiencies, measured and reconstructed*

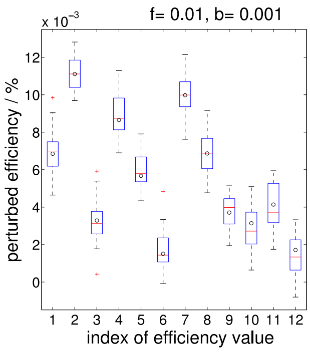


Fig. 9: *Randomly generated measurement values*

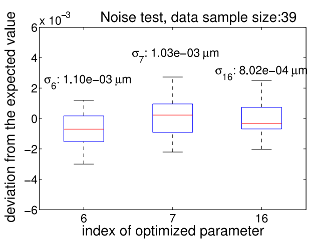


Fig. 10: *Distribution of parameters, deviations*

of $\mathcal{J}^\top \mathcal{J}$. The minimal eigenvalue should be maximized to avoid ill-posed mappings $(p_j) \mapsto (E_m)$, where small measurement uncertainties cannot be handled anymore. Additionally, a large minimal eigenvalue leads to small statistical confidence sets for the reconstructed solution. On the other hand, the maximal eigenvalue should be minimized to avoid cases where $(p_j) \mapsto (E_m)$ changes rapidly, such that the functional Φ might have many oscillations and many local minima.

Finally, suppose we have fixed the number of measurements M we are willing to employ in our scatterometric setup. To get the "best choice" of measurements is equivalent to choosing that subset of M efficiencies E_m for which κ takes the smallest value. Actually, the Jacobian matrix $\mathcal{J}$ in the definition of κ should be taken for the solution vector (p_j^{sol}). However, since the solution is not known beforehand, and since the numerical algorithm might pass through iterative solutions spread over a larger domain of vectors, we recommend to compute the κ at many vectors of the domain and to minimize the maximum of these κ values with respect to all choices of measurement subsets. Of course, if the number of all possible subsets is too large, then an optimization in an acceptable time is not realistic. In this case, the optimal subset should be replaced by an approximately optimal subset obtained by some sort of greedy algorithm; cf. [3]. We have presented approximately optimal measurement subsets and the corresponding results of the reconstruction algorithm for EUV line-space structures in [4].

For a number of $M = 12$ measurement values and for the reconstruction of the parameters p_j, $j = 2, 6, 7$ (see Figure 4), we have determined an optimal choice of efficiencies. Using this setup, we have reconstructed the three parameters optimizing the least-squares functional Φ. Figure 8 shows the measured reflection efficiencies and the efficiencies corresponding to the geometry with the three reconstructed parameters.

Estimation of reconstructed data

The measured efficiency values entering the numerical algorithm have special measurement uncertainties. So it is important to see how these uncertainties affect the reconstructed values. Apart from a background noise, the deviations of the measurement values from the true numbers are assumed to be proportional to the true numbers. Accordingly, using a random number generator, different series of measurements can be simulated (see the range of measurement values in Figure 9), and the corresponding parameters can be reconstructed. The resulting range of parameter values (see Figure 10) indicates the uncertainty of reconstruction. Such an approach is called *Monte Carlo method*.

Alternatively, a faster way to estimate the uncertainties is to follow a proposal by Al-Assaad and Byrne. Assuming the parameters to depend on the measured efficiency values in a simple manner, the parameter uncertainties can be determined from an approximate formula for the so-called *covariance matrix*. Numerical tests for an EUV line-space structure and for measurement uncertainties like in Figure 9 show a good agreement of the estimates based on the covariance matrix with those determined by the Monte Carlo method (see Table 1).

nmb. M of meas. / stand. dev.	12	415
$\sigma_2 = \sigma_{16}$ [nm]	0.91	0.15
σ_6 [nm]	0.81	0.012
σ_7 [nm]	0.86	0.054
σ_{SWA} [°]	1.3	0.14

Table 1: *Estimated standard deviations for reconstructed parameters*

Acknowledgment: The research was supported as part of the project ABBILD of the BMBF.

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2.2 The Storage Problem of Rechargeable Lithium-Ion Batteries

Wolfgang Dreyer

Background and objectives

Rechargeable lithium-ion batteries have become the most promising devices to convert chemical energy into electrical energy because they currently already offer 900 kilojoule per kilogram with a maximum power of 3,000 watt per kilogram. In this regime, the only competitors of lithium-ion batteries are fuel cells. However, there are various indications that the latter will loose the race due to high costs and their durability.

The primary functional components of a lithium-ion battery are the anode, the cathode, and an electrolyte. The choice of the materials for these components is of crucial importance concerning the voltage, the capacity, i.e., the total available charge per kilogram, and the lifetime of the battery, which rely sensitively on the reversibility of the charging/discharging process.

The usage of iron phosphate for the cathode is related to various dramatic call-back actions. For example, the mid-2006 recall of approximately 10 million Sony batteries was due to possible overheating, and it was even reported that some of them burst into flames. In those batteries, the cathode material is cobalt oxide. It is known that the substitute iron phosphate is not as sensitive to temperature. However, due to its storage capability, batteries with iron phosphate cathodes currently can store only about 75 percent of the energy that the cobalt oxide host system can store.

The process by which chemical energy is converted into electrical energy relies on the phenomenon that there exist pairs of atoms or molecules or complex compounds where one pair member donates electrons to the other member. These pairs can be read off from the electrochemical potential series, which orders the substances according to their property to donate or to accept electrons to or from the other members of the series. A member of the series may donate electrons to all members on its right-hand side and accept electrons from all members that are on its left-hand side. Thus, any pair of members of the electrochemical potential series can be used to convert chemical into electrical energy. The obtainable voltage depends on the distance between the two partners in the electrochemical potential series, which starts on its left-hand side with the element lithium, and for this reason, lithium is the most powerful candidate to form a pair.

In a rechargeable battery, both the anode and cathode do not directly take part in the electrochemical process that converts chemical energy into electrical energy; rather, they act as host systems for the element, which is here lithium, that donates the electrons for the external circuit.

In the following, we shall describe and exploit a mathematical model that is capable to capture the phenomena inside an iron phosphate cathode. For experimental tests of the cathode, usually, the anode is made of metallic lithium. However, it is important to note that a device containing an anode made of metallic lithium is not rechargeable, because the anode irreversibly dissolves during the discharging process so that its geometric shape cannot be recovered.

The arrangement shown in Figure 1 roughly indicates the processes in a lithium battery during discharging and charging. During discharging, electrons leave the anode to travel through an outer circuit. The remaining positive lithium ions leave the anode and move through an electrolyte towards the cathode, which is the central object of the current modeling. It consists of a carbon-coated single crystal $FePO_4$ with the shape of a small sphere of about 50 nm diameter. The $FePO_4$ lattice offers interstitial lattice sites that serve to store lithium atoms.

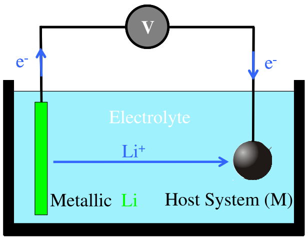


***Fig. 1:** Basic constituents of a rechargeable lithium ion battery for cathode testing*

When the battery is fully charged, all interstitial lattice sites are empty. During discharging, the arriving lithium ions combine at the carbon-coated surface of the $FePO_4$ ball with the inflowing electrons, and hereafter, they occupy the interstitial lattice sites. After complete discharging, a maximal number of sites of the interstitial lattice is occupied by lithium atoms. During recharging of the battery, the reverse process takes place.

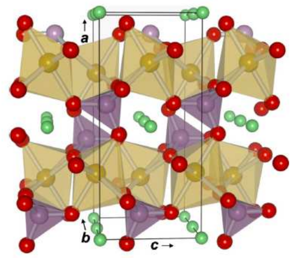


***Fig. 2:** $FePO_4$ crystal structure and interstitial lattice sites. Yellow: Fe, purple: P, red: O, green: interstitial lattice sites. From [3].*

Thermodynamic description of the host system

Constitution of the host system. The crystal lattice of the host system and, in particular, its mechanical properties are described in detail by T. Maxisch and G. Ceder in [3]. According to Figure 2, the lattice sites of the undeformed crystal have orthorhombic symmetry, and they are occupied by the iron phosphate units $FePO_4$. Furthermore, there is an interstitial sublattice whose lattice sites are completely empty, i.e., occupied by vacancies, in the undeformed state. To each unit of $FePO_4$ there corresponds one single site in the sublattice. Now Li atoms can be supplied or removed through the external boundary of the host system, and they will reside on the sublattice sites. The process of insertion of Li atoms is called lithiation.

The insertion of Li atoms into the host system leads to a deformation of the crystal lattice because a Li atom needs more space than a vacancy, and we observe a considerable change of the crystal volume. Additionally, the elastic stiffness coefficients change.

At room temperature, there exists a region of total Li concentration where the distribution of Li atoms on the sublattice sites is realized by two coexisting phases that differ by high and small Li concentrations. Our model is designed to describe an arbitrary morphology; however, our first numerical tests of the model rely on the simple geometry that is shown in Figure 3.

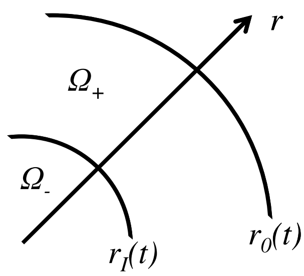


***Fig. 3:** The two-phase morphology of the host system*

Basic variables of the model. The host system consists of three constituents: there are $FePO_4$ units (M), generating the deformable matrix lattice. Furthermore, we have Li atoms (Li) and vacancies (V) on the sublattice. The number densities n_{M}, n_{Li}, and n_{V} of these constituents and the displacement vector $u = (u^i)_{i=1,2,3} = (u^1, u^2, u^3)$ of the deformable lattice are the basic variables. The free boundaries are described in the simplified model by the radii of the interface and the outer boundary, r_{I} and r_0.

The model's objective is to determine the evolution of the functions $n_{\mathrm{M}}(t,x)$, $n_{\mathrm{Li}}(t,x)$, $n_{\mathrm{V}}(t,x)$, $u(t,x)$, $r_{\mathrm{I}}(t)$, and $r_0(t)$ in time $t \geq 0$ and space $x = (x^i)_{i=1,2,3} = (x^1, x^2, x^3) \in \Omega$ by an initial and free boundary value problem.

Capacity, voltage, chemical potentials, and diffusion flux. For given capacity $C(t)$, the voltage

$U(t)$ of a lithium-ion battery cell can be experimentally measured, whereby the capacity gives the ratio of the total charge at time t and the weight of the cathode. On the other hand, for given Li flux $j_{\rm Li}(t, r_0(t))$ at the outer boundary, the solution of the described initial and free boundary value problem allows to calculate chemical potentials $\mu_{\rm Li}$ and $\mu_{\rm V}$. These quantities are related to the experimentally controlled quantities by

$$U(t) = -\frac{1}{e}(\mu_{\rm Li}(t, r_0(t)) - \mu_{\rm V}(t, r_0(t)) + U_0 \quad \text{and} \quad C(t) = -e\int_0^t j_{\rm Li}(\tau, r_0(\tau))d\tau, \qquad (1)$$

where $e = 1.6\ 10^{-19}\mathrm{As}$ is the charge of an electron, and $U_0 = 3.6\ \mathrm{V}$ is the potential of metallic Li.

Local conservation laws of particle numbers. The evolution of the three densities relies on the conservation laws of particle numbers, which read in regular points

$$\frac{\partial n_{\rm M}}{\partial t} + \mathrm{div}(n_{\rm M} v_{\rm M}) = 0, \quad \frac{\partial n_{\rm Li}}{\partial t} + \mathrm{div}(n_{\rm Li} v_{\rm Li}) = 0, \quad \frac{\partial n_{\rm V}}{\partial t} + \mathrm{div}(n_{\rm V} v_{\rm V}) = 0, \qquad (2)$$

and across the interface, there are the three jump conditions

$$-w^\nu[[n_{\rm M}]] + [[n_{\rm M} v^\nu_{\rm M}]] = 0, \quad -w^\nu[[n_{\rm Li}]] + [[n_{\rm Li} v^\nu_{\rm Li}]] = 0, \quad -w^\nu[[n_{\rm V}]] + [[n_{\rm V} v^\nu_{\rm V}]] = 0. \qquad (3)$$

Here, we have the velocities $v = (v^i)_{i=1,2,3} = (v^1, v^2, v^3)$ of the constituents: $v_{\rm M}(t,x)$, $v_{\rm Li}(t,x)$, and $v_{\rm V}(t,x)$, the normal speed w^ν of the interface with unit normal ν, and the double brackets indicate discontinuities across the interface.

The matrix lattice is fully occupied by the $FePO_4$ units, so that $n_{\rm M}(t,x)$ exclusively changes due to the lattice deformation. On the sublattice we may have diffusion, which, however, is restricted by the side condition that matrix lattice and sublattice have an equal number of lattice sites, thus we have $n_{\rm M}(t,x) = n_{\rm Li}(t,x) + n_{\rm V}(t,x)$. For this reason, we relate the velocity of the matrix $v_{\rm M}$ to the other velocities by $n_{\rm M} v_{\rm M}(t,x) = n_{\rm Li} v_{\rm Li}(t,x) + n_{\rm V} v_{\rm V}(t,x)$. This choice guarantees that the three local conservation laws of particle numbers reduce in a simple manner to only two independent conservation laws.

Local conservation laws of momentum. The evolution of the displacement vector $u = (u^i)_{i=1,2,3} = (u^1, u^2, u^3)$ relies on the conservation laws of momentum. Ignoring elastic waves, these conservation laws reduce to quasi-static force balances, and we may write in regular points of Ω, respectively, across the interface

$$\mathrm{div}\,\sigma = 0 \quad \text{and} \quad [[\sigma^{ij}]]\nu^j = -2\gamma k_M \nu^i. \qquad (4)$$

$\gamma > 0$ is the surface tension, and k_M denotes the mean curvature, which reads in polar coordinates for a sphere $k_M = -1/r_{\rm I}$. The quantity $\sigma = (\sigma^{ij})_{i,j=1,2,3}$ is the Cauchy stress tensor with $\sigma^{ij} = \sigma^{ji}$.

The detailed description of motion, strain, and stresses is given in [1]. Here, we describe a simplified mechanical model that ignores (i) the orthorhombic symmetry and (ii) the deviatoric stresses so that the stress tensor reduces to a pressure p: $\sigma^{ij} = -p\delta^{ij}$.

The second law of thermodynamics. The system of partial differential equations (PDEs) is closed by a constitutive model for the host system. It is shown by Dreyer et al. [1] that the knowledge of the specific free energy ψ is sufficient to give all needed constitutive quantities as functions of the variables:

$$\psi = \hat{\psi}(T, n_{\mathrm{Li}}, n_{\mathrm{V}}, c^{ij}) = \tilde{\psi}(T, y, \rho, c^{ij}) = \check{\psi}(T, y, C^{ij})\,. \tag{5}$$

The newly introduced quantities are the atomic fraction $y = n_{\mathrm{Li}}/(n_{\mathrm{Li}} + n_{\mathrm{V}})$, the mass density $\rho = m_{\mathrm{Li}}n_{\mathrm{Li}} + m_{\mathrm{M}}n_{\mathrm{M}}$, the right Cauchy–Green tensor $C = (C^{ij})_{i,j=1,2,3} = (1 + \mathrm{grad}(u))^T(1 + \mathrm{grad}(u))$, and its reduced form c with $\det(c) = 1$.

The calculation of the chemical potentials and of the pressure relies on the rules

$$\mu_{\mathrm{Li}} = \frac{\partial \rho\hat{\psi}}{\partial n_{\mathrm{Li}}}, \quad \mu_{\mathrm{V}} = \frac{\partial \rho\hat{\psi}}{\partial n_{\mathrm{V}}}, \quad p = \rho^2\frac{\partial\tilde{\psi}}{\partial\rho}, \quad \rho\psi + p = \mu_{\mathrm{Li}}n_{\mathrm{Li}} + \mu_{\mathrm{V}}n_{\mathrm{V}}, \tag{6}$$

and the function $\check{\psi}(T, y, C^{ij})$ is used to calculate the stress by means of

$$\sigma^{ij} = 2\rho\,(\delta^{im} + \frac{\partial u^i}{\partial x^m})(\delta^{jn} + \frac{\partial u^j}{\partial x^n})\frac{\partial\check{\psi}}{\partial C^{mn}}. \tag{7}$$

The evolution of the host system is controlled by two inequalities that give the entropy production in each point of the bulk phases, respectively, across the interface. They are formed by products of the type *flux* $\times$ *driving force*. In the bulk phases, the flux is the diffusion flux of the Li atoms, and the driving force here is given by the gradient of a chemical potential difference:

$$-j_{\mathrm{Li}}\nabla(\mu_{\mathrm{Li}} - \frac{m_{\mathrm{Li}} + m_{\mathrm{M}}}{m_{\mathrm{M}}}\mu_{\mathrm{V}}) \geq 0. \tag{8}$$

Across the interface, we have two products. The flux of the first product is the atomic Li flux across the interface $\dot{\mathcal{N}}_{\mathrm{Li}} = n_{\mathrm{Li}}(v_{\mathrm{Li}} - w^{\nu})$, and the driving force consists of the jump of a chemical potential difference plus a term containing the stress deviator, and the second product concerns the vacancy flux across the interface and a corresponding driving force:

$$\dot{\mathcal{N}}_{\mathrm{Li}}[[\mu_{\mathrm{Li}} - \mu_{\mathrm{V}} - \frac{m_{\mathrm{Li}}}{\rho}\sigma^{<ij>}\nu^i\nu^j]] + \dot{\mathcal{N}}_{\mathrm{M}}[[\mu_{\mathrm{V}} - \frac{m_{\mathrm{M}}}{\rho}\sigma^{<ij>}\nu^i\nu^j]] \geq 0. \tag{9}$$

The equality sign holds in equilibrium, where the entropy production assumes its minimum value zero. In non-equilibrium, the production of entropy must be positive.

The simplest possibility to satisfy the entropy inequality in non-equilibrium is given by Fick's law

$$j_{\mathrm{Li}} = -M_B\nabla(\mu_{\mathrm{Li}} - \frac{m_{\mathrm{Li}} + m_{\mathrm{M}}}{m_{\mathrm{M}}}\mu_{\mathrm{V}}), \tag{10}$$

where the bulk mobility satisfies $M_B(T, y) > 0$.

In analogy, we may read off from (9) so-called *kinetic relations* of the same formal structure as it is given by (10)

$$\dot{\mathcal{N}}_{\mathrm{Li}} = M_I^{\mathrm{Li}}[[\mu_{\mathrm{Li}} - \mu_{\mathrm{V}} - \frac{m_{\mathrm{Li}}}{\rho}\sigma^{<ij>}\nu^i\nu^j]], \tag{11}$$

$$\dot{\mathcal{N}}_{\mathrm{M}} = M_I^{\mathrm{M}}[[\mu_{\mathrm{V}} - \frac{m_{\mathrm{M}}}{\rho}\sigma^{<ij>}\nu^i\nu^j]]. \tag{12}$$

There are two interface mobilities $M_I^{\mathrm{Li}} > 0$ and $M_I^{\mathrm{M}} > 0$.

Limiting cases. The evolution of the host system is controlled by the three appropriately chosen mobilities. There are two interesting limiting cases. If the bulk mobility is considerably smaller than the interface mobilities, we may consider the limiting case $M_I^{\mathrm{Li}},\ M_I^{\mathrm{M}} \to \infty$. In this case, the jump brackets in (11), (12) must be zero, and serve as generalized Gibbs–Thomson laws. On the other hand, if the bulk mobility is considerably larger than the interface mobilities, we may consider the case $M_B \to \infty$. Then, the particle densities are homogeneous in the bulk phases, and the evolution of the host system is controlled by a system of ordinary differential equations. In the following, we shall exclusively consider this case.

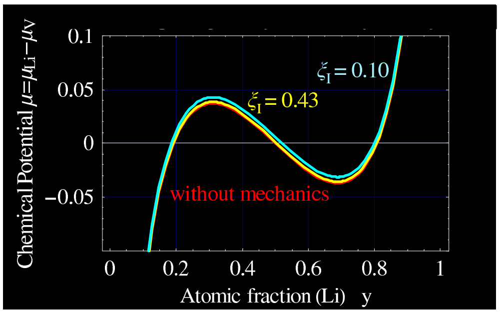
Simulations

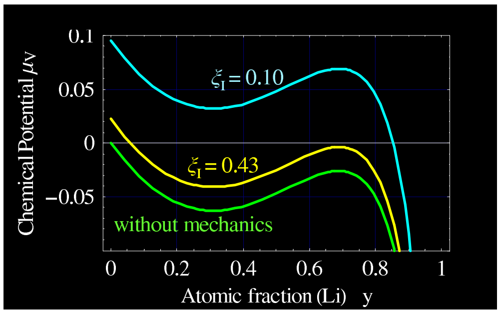
Chemical potentials. The chemical potentials $\mu = \mu_{\mathrm{Li}} - \mu_{\mathrm{V}}$ and μ_{V} and particularly their discontinuities across the interface determine the possible equilibria and, in combination with the two relaxation times, the evolution of the host system for given initial and boundary data.

Figure 4 illustrates both potentials, without and with mechanical contributions, that are due to surface tension and Li-induced volume changes of the matrix lattice. If these two phenomena were ignored, the chemical potentials would be represented by a function f that would depend exclusively on the Li fraction y: $\mu = f'(y)$ and $\mu_{\mathrm{V}} = f(y) - yf'(y)$. Thus in this case, the chemical potentials are given by the red and green curve of Figure 4, respectively.

If the mechanical phenomena are taken into account, the chemical potentials additionally depend on the radius of the interface, i.e., on ξ_{I}. This dependence is illustrated in Figure 4 by the yellow and blue curves, which give the chemical potentials μ and μ_{V} for the two radii $\xi_{\mathrm{I}} = 0.43$ and $\xi_{\mathrm{I}} = 0.10$.

Fig. 4: Yellow and blue: chemical potentials with mechanical contributions for two different interfacial radii. Red and green: without mechanical contributions.





Finally, it is important to note that the non-monotonicity of the chemical potentials induces an ill-posed problem if we consider the nonhomogeneous diffusion problem because regions with negative diffusion coefficients will appear. However, that ill-posedness can be removed by a regularization of the PDE system.

Possible equilibria. For given total fraction q of stored Li atoms, we now determine the possible equilibria (y^+, y^-, ξ_I), which rely on the algebraic system

$$\mu^+ = \mu^- \quad \text{and} \quad \mu_V^+ = \mu_V^-, \tag{13}$$

and on a so-called *Stefan condition* that is obtained from the interfacial particle conservation laws (3). After its integration, we end up with a third algebraic equation.

If we ignore the mechanical contributions, these equations reduce to the classical common tangent construction

$$f'(y^+) = f'(y^-) \quad \text{and} \quad f(y^+) - y^+ f'(y^+) = f(y^-) - y^- f'(y^-), \tag{14}$$

which determine the so-called *Maxwell line*. In this case, the solution of (y^+, y^-) to (14) exhibits a symmetry because we may have $y^+ > y^-$ as well as $y^+ < y^-$. A variation of the location of the interface does not change the equilibrium. After (14) is solved for (y^+, y^-), we may use the integrated Stefan condition to determine for given q the interface radius ξ_I.

If we now include the mechanical phenomena into the discussion of the system (13), the radius ξ_I of the interface appears in these equations, and thus the equilibria (y^+, y^-) depend on ξ_I. There are two different compact domains of radii so that the triple (y^+, y^-, ξ_I) solves the equations (13) and the integrated Stefan condition. The first domain contains the radii for which we have $y^+ > y^-$, while in the second domain $y^+ < y^-$. There is no symmetry anymore between the outer and inner region of the host system.

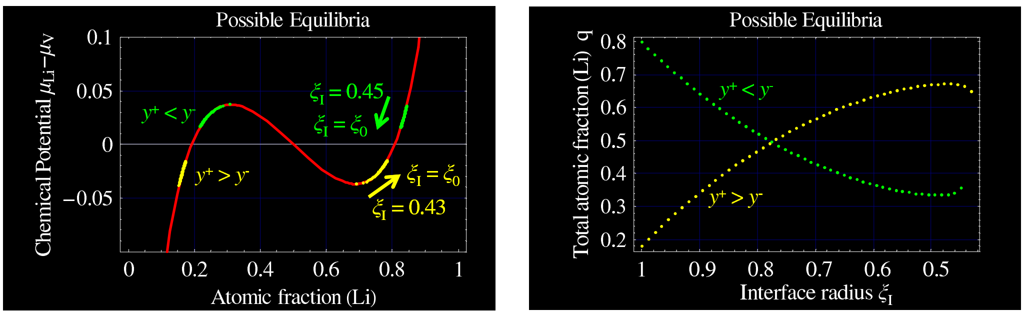


Fig. 5: *Possible equilibria when mechanical contributions are taken into account. Left:* $\mu = \mu_{Li} - \mu_V$ *and possible equilibria* (y^+, y^-) *for* $y^+ > y^-$ *(yellow) and for* $y^+ < y^-$ *(green). Right : the corresponding interfacial radii* ξ_I *for given fixed total Li fraction.*

From the left plot of Figure 5, we may read off the possible atomic Li fractions in equilibrium, which are indicated by dots in yellow color for $y^+ > y^-$, and in green color for $y^+ < y^-$.

The plot on the right-hand side gives the corresponding interfacial radii for given total atomic Li fractions. It is important to note that for given q there is a region where two equilibria are possible. The third possibility for small ξ_I corresponds to a saddle point of the free energy. Which one is assumed by the host system for given initial data depends on the ratio of the relaxation times.

Hysteretic behavior. If the host system approaches interfacial equilibrium on a much faster time scale than the loading or the unloading process, respectively, then the model predicts a hysteretic behavior of the host system. This fact can be read off from the data given in Figure 5 that are now used to construct the graph $-\mu^+ = -(\mu_{Li}^+ - \mu_V^+)$ versus the total Li content of the host system, $1-q$. By means of (1), $-\mu$ and $1-q$ are related to voltage and capacity, respectively, so that the voltage/capacity plot exhibits a hysteresis.

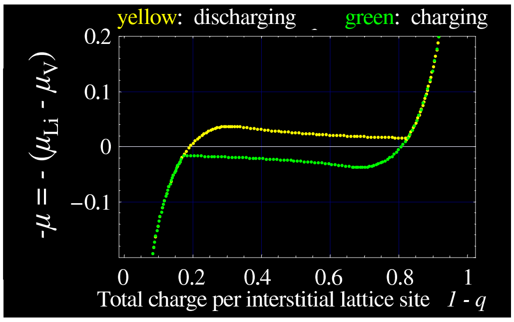


Fig. 6: *Hysteretic behavior during charging (green) and discharging (yellow)*

On the flexibility of mathematical models

The described model is not restricted to the simulation of the storage problem of a rechargeable lithium-ion battery. There are two further important applications.

Hydrogen is the ideal synthetic fuel to convert chemical energy into electrical energy or into motive power because it is lightweight, highly abundant, and its oxidation product is water vapor. One possibility to store hydrogen is similar to the case from above because also here crystal lattices of metals or other compounds can be used as the storage system, where hydrogen is dissolved by substitution either on interstitial or on regular lattice sites. The latter process and its reversal is called *hydriding* and *dehydriding*, respectively. Even a phase transition with two coexisting phases also occurs during the processes of hydriding and dehydriding. For small partial pressure, which is accompanied by a small hydrogen fraction, the hydrogen atoms form a single *solid solution*. Above a certain pressure, the appearance of a so-called *hydride phase* sets in, and the pressure/hydrogen fraction plot shows likewise a hysteretic phenomenon.

A further application of the model concerns the austenite-ferrite phase transition in steel [2], where the amount of carbon, which resides on interstitial lattice sites, controls the lattice symmetry of the iron lattice, i.e., the austenite and ferrite phase, respectively.

Thus, currently there are three different applications for the same mathematical structure.

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2.3 Mass-conservative Scott–Vogelius Discretization for the Incompressible Navier–Stokes Equation

Alexander Linke

Many phenomena in science and industry depend on movements of liquids and transport and reaction of dissolved species therein. This includes typical thin-layer flow-cell experiments in electrochemistry, where dissolved species in a liquid react at a catalyst. These experiments elucidate the heterogeneous catalytic reactions taking place in fuel cells, see Figure 1. Numerical simulation helps to interpret these experiments. The numerical challenge is the complex interaction between liquid flow, transport, diffusion, and reaction phenomena.

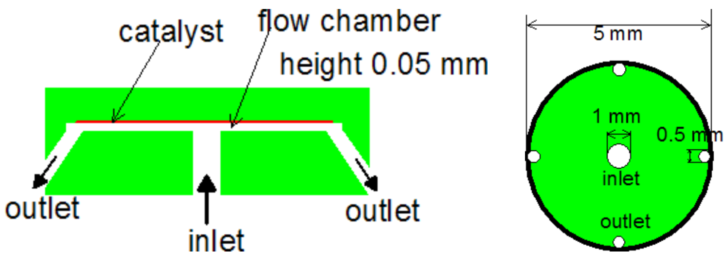


***Fig. 1:** Thin-layer flow cell. Catalytic reactions occur at the top of the working chamber. Left: section. Right: top view*

Continuum mechanics

Transport, diffusion, and reaction processes in liquids are described by classical models from continuum mechanics. Numerical mathematics has developed various methods for their numerical simulation on modern computers. Provided the behavior of a liquid flow is known, accurate and stable simulation methods for reaction, diffusion, and transport processes are at hand; see [1]. Unfortunately, the simulation of the liquids themselves remains a challenging task. Liquids are described by the famous incompressible Navier–Stokes equation, formulated about 150 years ago. There exists an uncountable number of simulation methods for this equation. The reason for this is a number of different possible instabilities, spoiling the accuracy of numerical simulations. In this article, we focus on weak mass conservation, an instability seemingly underestimated and hardly understood in Navier–Stokes simulations. We present the Scott–Vogelius finite element method solving the arising problems, and illustrate its practical use in applications.

The incompressible Navier–Stokes equation

The incompressible Navier–Stokes model describes the time evolution of a velocity field $\vec{u}(t, \vec{x})$ and a pressure field $p(t, \vec{x})$ within a liquid:

$$\vec{u}_t - \frac{1}{Re}\Delta \vec{u} + (\vec{u} \cdot \nabla)\,\vec{u} + \nabla p = \vec{f}$$
$$\nabla \cdot \vec{u} = 0.$$

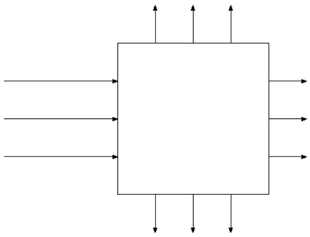


Fig. 2: *Local mass conservation: the inflow into the (quadratic) test volume balances the outflow. The length of the arrows indicates the velocity* $\vec{u}(t, \vec{x})$ *of the liquid*

The first equation describes the momentum conservation and models a force balance. The model includes frictional forces $-\frac{1}{Re}\Delta\vec{u}$, inertial forces $(\vec{u}\cdot\nabla)\vec{u}$, and forces due to pressure differences ∇p, as well as outer forces $\vec{f}$, e.g., gravitation. The second equation describes mass conservation and means that at every time t, the inflow of the liquid into an arbitrarily small test volume balances its outflow; see Figure 2. Mass-conservative liquid flows $\vec{u}$ are called *divergence free*, since the operator $\nabla\cdot$ is called *divergence operator*. The Reynolds number Re characterizes the complexity of a flow problem. The higher the Reynolds number, the larger the inertial forces compared to the frictional forces, and the larger the problems for numerical simulation, too. A typical Reynolds number for flow-cell experiments in electrochemistry is 100. But already the flow excited by a human swimmer can have Reynolds numbers up to 4,000,000.

Discretization methods for incompressible flows

For the numerical simulation of liquid flows, various methods have been developed. Numerical approximations use a finite number of *degrees of freedom* and allow to assemble a series of equations approximating the physics of the flow problem, i.e., its geometry and outer forces $\vec{f}$. This is called the *discretization* of the problem, since an infinitely-dimensional continuum model is reduced to a finite-dimensional discrete one. The more precise the numerical simulation is desired to be, the more degrees of freedom are necessary. Then, time and memory requirements increase similarly. Discretization methods for the incompressible Navier–Stokes equation must approximate mass conservation and momentum conservation at the same time. It is not possible to fulfill exact momentum conservation in a discretization method. Instead, we must use ever more degrees of freedom in order to approximate momentum conservation with a tolerable accuracy. Similarly, most discretization methods only approximate mass conservation, although it is exactly achievable. The Scott–Vogelius mixed finite element method is such a method.

Instabilities due to weak mass conservation

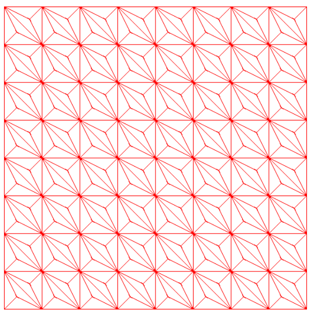


Fig. 3: *Mesh for* no-flow example

Inaccurate mass conservation is a possible source for instabilities in numerical computations. It can decrease the accuracy of simulations significantly. An academic, but telling example illustrates this. We compare two different conforming Galerkin mixed finite element discretizations for the incompressible Navier–Stokes equation, the popular Taylor–Hood element, and the hardly-known Scott–Vogelius element; see [2]. Both methods use the same discretization for the velocity. But their pressure discretization is different. We solve a two-dimensional Navier–Stokes problem at three different Reynolds numbers $Re \in \{1; 100; 1000\}$ with force vector $\vec{f} = (3x^2+1, 3y^2)^T$ and no-slip boundary conditions in a square domain; see Figure 3. Both discretizations use 1,602 velocity degrees of freedom. The Scott–Vogelius method uses 1,152 degrees of freedom for the pressure, while the Taylor–Hood methods needs only 209 pressure variables. The exact Navier–Stokes solution is $\vec{u} = \vec{0}$ and $p = x^3 + y^3 + x - 1$, independently of the Reynolds number Re, i.e., there is no flow. The role of the pressure is to balance the outer force vector $\vec{f}$. Both discretizations deliver three different approximative velocities, depending on the Reynolds number. For judging their quality, we compare the quadratic means of the error (L_2-error):

Re	$\|\vec{u}-\vec{u}_{approx,TH}\|$	$\|p-p_{approx,TH}\|$	$\|\vec{u}-\vec{u}_{approx,SV}\|$	$\|p-p_{approx,SV}\|$
1	$2.03\cdot 10^{-5}$	$2.37\cdot 10^{-3}$	0	$1.63\cdot 10^{-3}$
10	$2.03\cdot 10^{-4}$	$2.37\cdot 10^{-3}$	0	$1.63\cdot 10^{-3}$
100	$2.03\cdot 10^{-3}$	$2.37\cdot 10^{-3}$	0	$1.63\cdot 10^{-3}$
1,000	$2.03\cdot 10^{-2}$	$2.38\cdot 10^{-3}$	0	$1.63\cdot 10^{-3}$

Table 1: *Quality of Galerkin Taylor–Hood and Galerkin Scott–Vogelius approximations in no-flow example*

Both discretizations produce comparable approximations for the pressure p, independent of the Reynolds number. But the velocity discretizations differ. Here, the Taylor–Hood element delivers an error proportional to the Reynolds number, i.e., it is an instable discretization. Instead, the Scott–Vogelius discretization is error free. The consequences for computer resources like memory and time are dramatic. In order to achieve an accuracy of $1.63\cdot 10^{-5}$ at Reynolds number 1 with the Taylor–Hood element, we need about 1,600 velocity degrees of freedom. But at Reynolds number $Re=$ 1,000, we need a factor of $Re^{2/3}=100$ times more degrees of freedoms for that. In 3D, the factor is $Re=$1,000. This is a serious problem for numerical computations. But why does the instability occur only with the Taylor–Hood element? The answer can be understood by a geometrical analogy. Solutions of the incompressible Navier–Stokes equation are divergence free. But also the force vector $\vec{f}=(3x^2+1,3y^2)^T$ has a special structure. It is *rotation free*. Divergence-free and rotation-free velocities are perpendicular in some sense (w.r.t. the L^2 scalar product), and this assures $\vec{u}=\vec{0}$ in the no-flow example. This holds also for the divergence-free Scott–Vogelius element. But Taylor–Hood velocities possess only an approximate mass conservation. They are not divergence free and are not perpendicular to $\vec{f}$. Therefore, the rotation-free vector $\vec{f}$ spoils the Taylor–Hood approximation $\vec{u}_{approx,TH}$.

Mass conservation and transport

Now, we assume that some species is dissolved within the incompressible fluid. The distribution of its concentration is modeled by a convection-diffusion equation. This model possesses mathematical properties like positivity of the concentrations and different maximum principles. Therefore, concentrations are always limited to their values on the boundary. Such a maximum principle holds provided the velocity is divergence free. There exist successful numerical discretizations of convection-diffusion equations, which can guarantee positivity and maximum principles also for discrete approximations, provided the discrete velocity is divergence free, e.g., the Voronoi box based finite volume scheme. Such analogous discrete results are especially important when nonlinearities occur. Here, the divergence-free Scott–Vogelius discretization rescues the important maximum principle when the discrete velocity is coupled to a finite volume scheme for convection-diffusion equations; see Figure 4 and [4].

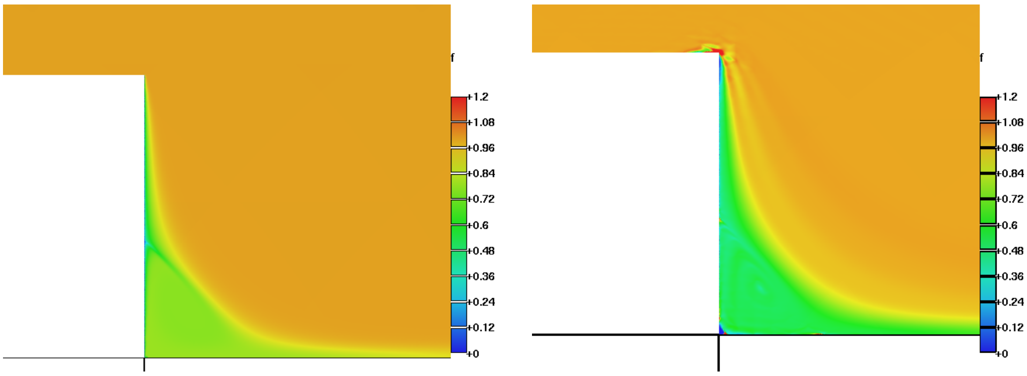
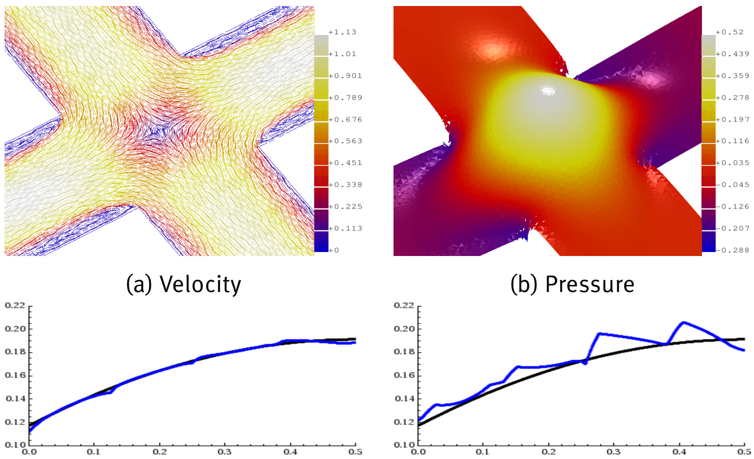


Fig. 4: *Finite volume discretization for transport and diffusion in a liquid flow. Left: divergence-free Scott–Vogelius element assures that concentrations are in* $[0,1]$. *Right: Taylor–Hood element destroys maximum principle*

Mass conservative or not mass conservative

Looking at Table 1 and Figure 4, we ask: why is the Taylor–Hood element popular and Scott–Vogelius is not? First, a practical Scott–Vogelius method in 3D has been proposed only in 2005, see [3], and in 2D, divergence-free velocities are cheaper to obtain by velocity-vorticity formulations. Second, exact mass conservation is not always needed, and it is not for free. Let us revise the no-flow example. Scott–Vogelius uses 1,602 degrees of freedom for the velocity and 1,152 degrees of freedom for the pressure. Unfortunately, only $1,602 - 1,152 = 450$ degrees of freedom are divergence free. Instead, Taylor–Hood uses 209 pressure degrees of freedom and applies $1,602 - 209 = 1,393$ velocity degrees of freedom for the approximation of a liquid flow. Often, this is an advantage. But the additional Taylor–Hood degrees of freedom are not divergence free and prone to instability. Numerical analysis indicates that instability due to weak mass conservation appears when the curvature of the pressure and the Reynolds number are large. In the no-flow example, this is the case. When we have $\vec{f} = \vec{0}$, it is more difficult to find examples where Scott–Vogelius beats Taylor–Hood. For such an example, see Figure 5 and [4].



(a) Velocity

(b) Pressure

(c) Coarse stable vertical Scott–Vogelius velocity (blue) and reference solution (black)

(d) Coarse instable vertical Taylor-Hood velocity (blue) and reference solution (black)

Fig. 5: *Colliding beams at Reynolds number* $Re = 1,024$, $\vec{f} = \vec{0}$: *two beams collide in the center of a cross domain. A large pressure develops and the divergence-free Scott–Vogelius element is more accurate than Taylor–Hood. The mesh is refined at the boundaries and the corners in order to prevent convective instabilities due to boundary layers*

Mathematical highlights of Scott–Vogelius elements

Finally, we highlight some mathematical properties of the Scott–Vogelius mixed finite element method. The Scott–Vogelius element uses P_k elements for the velocity and discontinuous $P_{-(k-1)}$ elements for the pressure. It is inf-sup-stable on quite general meshes, for $k \geq d$, with d the space dimension. Stability is assured by a macroelement construction; see [3], [4], and Figure 6. The Scott–Vogelius element delivers divergence-free pointwise velocities and therefore it is an *interior* mixed finite element method. The continuous pressure *does not influence at all* the discrete velocities $\vec{u}_h$. Dominant convection is stabilized by symmetric stabilization operators like the *continuous interior penalty* method, without destroying mass conservation; see [2], [4]. Discrete generalized Stokes problems can be solved by standard multigrid methods, since the cumbersome grad-div stabilization drops out. Also, the stabilization against dominant convection is included in the multigrid analysis; see [4], [5]. The coupled Scott–Vogelius/finite volume scheme was successfully used in a 3D simulation of thin-layer flow-cell experiments in electrochemistry; see Figure 7.

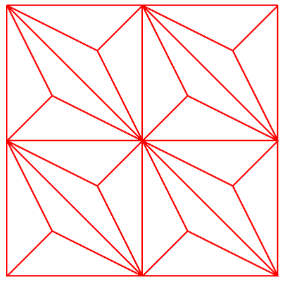


Fig. 6: *2D simplex mesh with 8 macro triangles*

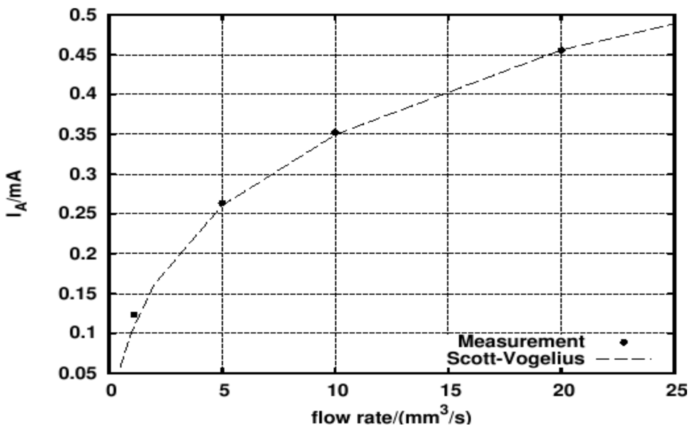


Fig. 7: *This flow-cell experiment determines the limiting current vs. the flow rate (with the catalytic reaction $H_2 \rightarrow 2H^+ + 2e^-$). The numerical simulation uses the Scott–Vogelius element for the incompressible 3D flow and a finite volume scheme for species transport and diffusion*

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2.4 Nonlinear Effects in Fiber Optics

Andrei G. Vladimirov, Uwe Bandelow, Ayhan Demircan, Monika Pietrzyk, Shalva Amiranashvili, and Mindaugas Radziunas

Photonic crystals have revolutionized research in optics and optoelectronics over the recent years. In particular, unique possibilities to manipulate the group velocity dispersion (GVD), i.e., the frequency dependence of the material refractive index, have become achievable with the invention of photonic crystal fibers (PCFs). These fibers are especially important for numerous applications, such as the generation of very intense white light, also known as supercontinuum, the construction of high-power fiber lasers, optical communications, ultrashort pulse generation, etc. Unlike pulses in standard telecom fibers, which are usually treated by keeping only the second-order term in the GVD Taylor expansion [1], taking into account higher-order dispersion is prerequisite for an adequate mathematical modeling of short optical pulse propagation in PCFs.

High-order dispersion in nonlinear optical fiber devices

Propagation of a short pulse through a nonlinear dispersive optical medium can result in considerable changes of its temporal and spectral properties (see Figure 1). For example, the supercontinuum generation in nonlinear fibers has been a subject of numerous investigations for years, due to very promising applications as a source of ultrabroad optical spectrum and interesting nonlinear mechanisms involved in the spectral broadening process. There is a variety of effects modifying the shape of a pulse and its spectrum. Among those are soliton fission associated with a break-up of a pulse into several smaller pulses (see Figure 1b) and, accompanied by the generation of dispersive waves, modulation instability (MI), leading to exponential growth of the pulse amplitude modulation ripples, Raman scattering, and other four-wave mixing processes.

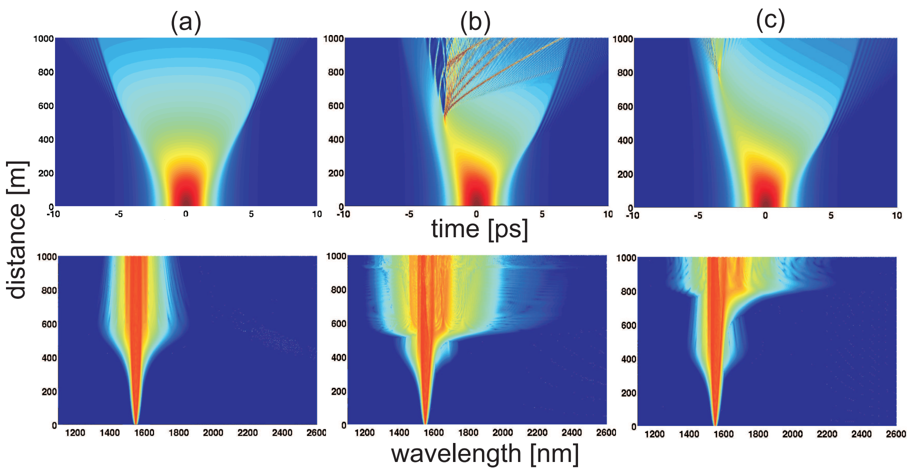

***Fig. 1:** Temporal (upper row) and spectral (lower row) evolution of a short optical pulse in the normal GVD regime: (a) only second-order dispersion β_2 is present, (b) $\beta_2, \beta_3 \neq 0$ and $\beta_4 = 0$, (c) $\beta_2, \beta_3, \beta_4 \neq 0$*

In [1], the extended nonlinear Schrödinger equation (NLSE) for the complex electric field envelope A:

$$\frac{\partial A}{\partial \zeta} = -\frac{i}{2}\beta_2 \frac{\partial^2 A}{\partial \tau^2} + \frac{1}{6}\beta_3 \frac{\partial^3 A}{\partial \tau^3} + \frac{i}{24}\beta_4 \frac{\partial^4 A}{\partial \tau^4} + i\gamma A|A|^2, \tag{1}$$

was analyzed numerically using a pseudospectral method. The impact of third- (β_3) and fourth- (β_4) order dispersion on the propagation of short optical pulses along highly nonlinear fibers was studied. It was shown that in the *anomalous GVD* regime ($\beta_2 < 0$), the MI and soliton fission drastically modify high-order soliton pulses and their spectra. Nonzero β_3 can induce soliton fission accompanied by nonsolitonic radiation and yields asymmetric spectra in general, whereas MI is slightly suppressed by the term proportional to β_4 in this regime. In the *normal GVD* regime ($\beta_2 > 0$), the initial spectral broadening of a pulse is dominated by self-phase modulation (the last term in Eq. (1)), whereas its further evolution strongly depends on the underlying fiber dispersion profile, which either allows for solitonic effects or prevents them. Pulse splitting has been demonstrated for $\beta_3 \neq 0$ (see Figure 1b), as well as its later suppression by the term proportional to β_4 (see Figure 1c).

Development of MI responsible for the short pulse formation in a coherently driven PCF cavity (see Figure 2) was modeled in [2] using Eq. (1) with an additional loss term $-\alpha A$ and an additional driving term $A_i \exp(i\omega\zeta)$ in the right-hand side. It was found that only even-order τ-derivatives in Eq. (1) contribute to the MI gain and that it is necessary to take them into account up to the β_4-term to capture the full MI dynamics. Furthermore, for $\beta_4 \neq 0$, the MI has a finite domain of existence delimited by two pump power values that allows for the state with stationary intensity to recover stability at large powers. Numerical simulations of the generalized driven damped NLSE performed for a realistic experimental configuration with a flattened dispersion photonic crystal fiber are in an excellent agreement with the analytical predictions.

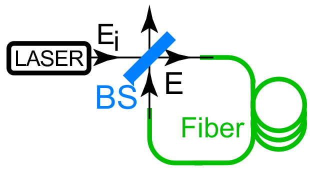

Fig. 2: *Externally driven PCF cavity.* E *– intracavity field,* E_i *– injected field, BS – beam splitter*

Spatial optical solitons in microstructured media

Modulational instability of discrete optical solitons in waveguide arrays. Although PCFs admit large degrees of the GVD engineering by periodic variations of the refractive index, diffraction is usually suppressed in these fibers. A simplest optical system that allows investigation of the functionality of the diffraction control is an array of coupled optical waveguides (Figure 3a). Such arrays can exhibit various nonlinear phenomena resulting from the interplay of strong nonlinearity and the so-called *discrete diffraction*, including the formation of stationary and moving "discrete" solitons, characterized by a nonlinear localization of light in a small number of waveguides. The theoretical investigation of waveguide arrays becomes particularly important now because of the advances in the fabrication of low-loss planar silicon-on-insulator structures with strong and controllable GVD and short coupling length, as well as multicore PCF (Figure 3b), having numerous promising applications.

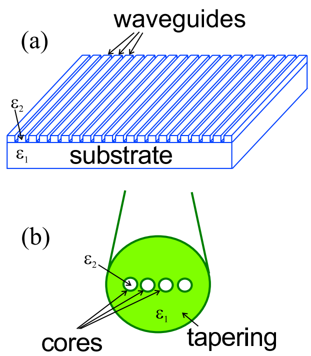

Fig. 3: *Planar waveguide array (a) and multicore PCF (b)*

Numerical modeling of the development of MI of bright discrete solitons in an array of coupled dispersive waveguides was performed in [3] using the set of coupled NLSEs

$$\frac{\partial A_k}{\partial \zeta} = -\frac{i}{2}\beta_2 \frac{\partial^2 A_k}{\partial \tau^2} + \frac{i}{2}\kappa \left(A_{k-1} + A_{k+1} - 2A_k\right) + i\gamma A_k|A_k|^2, \quad k = 1, \ldots, N. \tag{2}$$

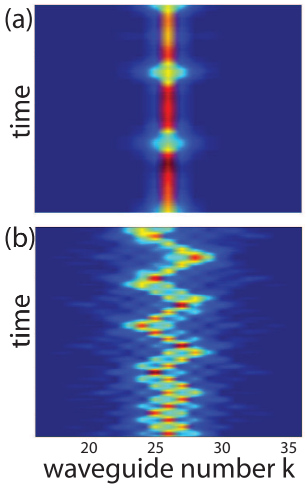

Fig. 4: *Discrete soliton breakup associated with* neck *(a) and* snake *(b) type of instability*

Here, A_k is the electric field envelope in k-th fiber and N is the number of fibers in the array. It was shown that, in the case of normal GVD, multiple instability bands exist in the frequency domain. For weak to moderate strength of coupling, the discrete solitons exhibit the so-called *neck instability* (see Figure 4a), leading to a breakup of the solitons into a train of dispersive pulses. Only for strong coupling, i.e., in the quasi-continuous limit, this instability is gradually suppressed by the so-called *snake instability* (see Figure 4b) known for the (2+1)D continuous NLSE model. In the case of the anomalous GVD, the expected *neck*-type instability leads to the formation of composite discrete-continuous spatio-temporal quasi-solitons (Figure 4a). The estimates for parameter values typical for SOI waveguides show that all the effects described in [3] are within the experimental reach, while dispersion-induced MI in a single silicon-on-insulator waveguide has already been reported in the literature.

Chaotic soliton walk in microstructured media. Recent developments in the fabrication of microstructured waveguiding materials have stimulated a growing interest in the investigation of nonlinear light beam propagation in various inhomogeneous settings. In particular, mobility properties of transverse spatial solitons were studied [4] in a situation where the refractive index of the medium is subjected to a weak periodic modulation in the plane orthogonal to the beam propagation direction. Using the Lyapunov–Schmidt reduction, ordinary differential equations were derived, which describe the soliton as a Newtonian particle in the external potential created by the refractive index profile. These equations remain valid independently of the ratio of the soliton transverse size to the modulation period, even when the soliton is quite wide.

Numerical simulations of the (2+1)D NLSE-type equation for the electric field amplitude A:

$$\frac{\partial A}{\partial \zeta} = i\left(\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial y^2}\right) + Af\left(|A|^2\right) + i\epsilon g(x,y)A \quad (3)$$

were performed with the help of a split-step pseudospectral method [4]. It was shown that a spatial soliton in a medium with a transverse modulation $g(x,y)$ of the refractive index can move both in a regular and a chaotic manner like a particle in a two-dimensional potential, and the choice between these two types of motion is foremost determined by the geometry of the refractive index profile.

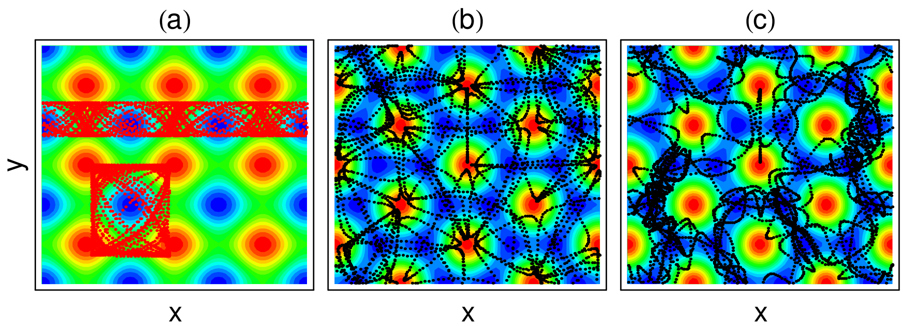

Fig. 5: *Quasiperiodic soliton trajectories in square lattice (a) and random trajectories of a conservative (b) and a dissipative (c) soliton in a hexagonal lattice*

When the refractive index $g(x,y)$ forms a rectangular lattice, the effective potential is integrable, and the soliton transverse motion is very close to an integrable one for long-time intervals (see

Figure 5a). There are two typical dynamical regimes in this case: (i) low-energy quasi-periodic oscillations around a local maximum of the refractive index and (ii) quasi-periodic oscillations superimposed on a constant velocity drift (see Figure 5a). In the case of a hexagonal lattice, the situation is drastically different. Here, with the increase of the soliton kinetic energy, the oscillations near a local maximum of the refractive index are transformed into a random walk, i.e., an unbounded transverse motion of the soliton wandering chaotically between different cells of the refractive index profile (see Figure 5b,c). This effect takes place both in the case of conservative and dissipative nonlinearity $f(|A|^2)$ and is of universal nature solely attributed to the Galilean symmetry group of the unperturbed Eq. (3).

Short pulse interactions in mode-locked fiber lasers

The problem of optical pulse interaction and bound-state formation is very important in the context of their applications in telecommunication technologies. On the one hand, the interaction implies strict limitations on the amount of information that can be transmitted, using the sequences of closely packed equidistant pulses. On the other hand, different bound states of optical pulses can serve as an "alphabet", suitable for increasing the density of the transmitted information.

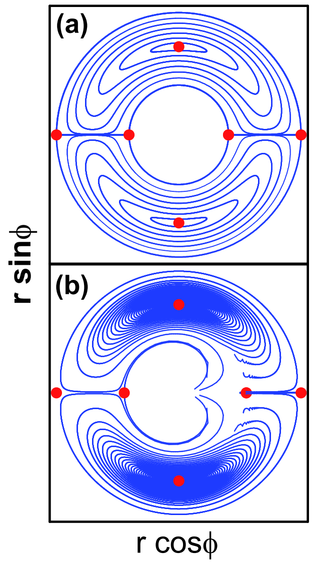

Fig. 6: Phase portraits for the two-pulse interaction in the unperturbed model obtained by (a) the solution of the PIE, (b) direct simulations of the QCGLE. r – distance between the pulses, ϕ – their phase difference. Red dots indicate the positions of pulse bound states.

In [5], the quintic complex Ginzburg–Landau equation (QCGLE) was used to model the interaction of short optical pulses in a mode-locked fiber laser. In a certain parameter range, the QCGLE exhibits a localized solution corresponding to a short optical pulse propagating along the laser cavity axis. Being well separated from one another, two pulses interact via their exponentially decaying tails. Interference between these tails can produce spatial intensity oscillations responsible for the formation of pulse bound states. For the case of weak pulse interaction, a set of ordinary differential pulse interaction equations (PIE) governing the slow time evolution of the pulse positions and phases was derived using the invariant manifold reduction method. Being independent of specific details of the model, the form of the PIE is determined only by the asymptotic behavior of the pulse tails and the symmetry properties of the model equations.

When the model equations admit only translational symmetry, PIEs have a gradient structure, which implies a trivial dynamics for the interacting pulses. The additional $U(1)$ (phase-shift) symmetry group of the QCGLE results in effectively two-dimensional interaction dynamics with simple attractors, corresponding to stationary or uniformly moving pulse bound states (see Figure 6). Thus, one could expect that the breakdown of the $U(1)$ symmetry would make the dynamics just simpler. On the contrary, as it is shown in [5], slight breaking of the $U(1)$ symmetry due to a weak external signal injected into the laser cavity can produce a huge variety of dynamic bound states, characterized by undamped regular or chaotic oscillations of the soliton's coordinates and phases. These asymptotic results are consistent with those obtained by direct numerical modeling of the QCGLE using the Crank–Nicholson scheme (see Figure 7) and a path-following algorithm to trace localized solutions.

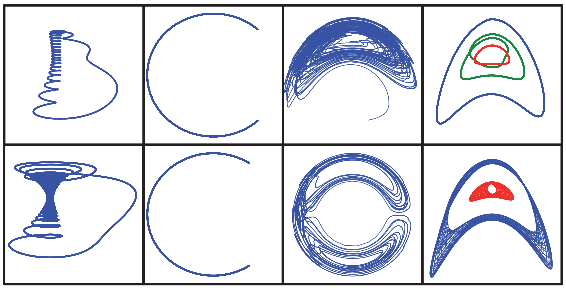

Fig. 7: *Phase trajectories for periodic and chaotic pulse interaction in the laser model with weak external injection: (a) direct simulations of the QCGLE, (b) numerical solutions of the PIE*

Formation and propagation of femtosecond optical pulses

Ultrashort optical pulses have numerous practical applications, including high bit-rate communications, optical tomography, spectroscopic measurements, material processing, frequency standards, etc. Of special importance is the investigation of few-cycle optical pulses with a temporal extent of less than a few cycles of the corresponding electromagnetic wave. Traditional approaches based on the slowly varying envelope approximation and resulting in NLSE-type equations are not suitable for the description of such pulses. Instead, the so-called *short pulse equation* (SPE):

$$\partial_z E - A\partial_\tau^3 E + B\int_{-\infty}^{\tau} E d\tau + CE^2\partial_\tau E = 0 \tag{4}$$

for the electric field E has been derived starting directly from the Maxwell equations.

Standard treatment of the fiber GVD in terms of a Taylor series expansion near the carrier frequency is also not valid for few-cycle pulses. Therefore, to describe ultrashort pulse propagation in a fluoride glass fiber in a wide spectral range, we have proposed a new SPE model based on the fitting of the actual dispersion function within a suitable interval of frequencies. This model predicts the existence of a family of uniformly moving solitary solutions preserving their shape. It has been shown that the classical envelope soliton appears with the increase of the total pulse duration as a limiting member of the family (see Figure 8). In the opposite limiting situation, one obtains the family member corresponding to the shortest and most intense pulse that can still propagate in a stable manner.

In order to take into account the optical anisotropy of real optical fibers, one needs to consider two polarization modes of the pulse. An appropriate two-component generalization of the SPE, including three integrable cases, has been developed in [6] by considering the zero-curvature representation of the matrix generalization of the SPE. This allowed to construct short pulse analogues of the coupled NLSE, known also as the *Manakov system*.

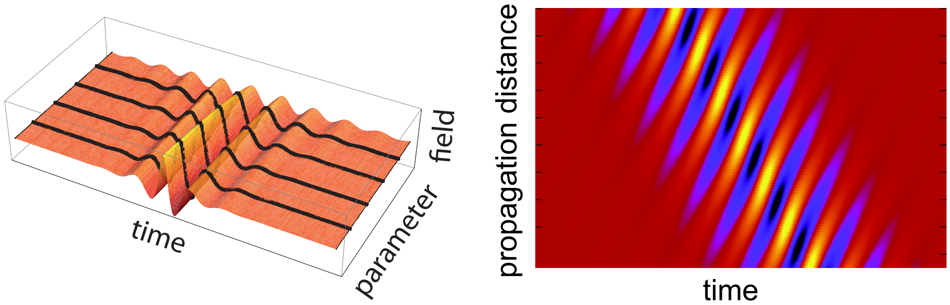

Fig. 8: *Left: ultrashort optical pulse shown for different values of the soliton family parameter. As the parameter increases, the pulse evolves to a standard envelope soliton. Right: spatio-temporal evolution of the ultrashort pulse solution of the SPE obtained with the help of the multisymplectic integrator*

Fast and stable numerical schemes for the numerical solution of the SPE and its generalizations were proposed in [7]. The key idea is to use a specific discretization, the multisymplectic integrator, which preserves the so-called *multisymplectic structure*. This techniques is a generalization of the technique of symplectic integrators to PDEs. Unlike the infinite-dimensional symplectic structure associated with PDEs, the multisymplectic structure is defined over a finite-dimensional analogue of the phase space. According to the results of [7], our multisymplectic integrator appears to be an order of magnitude more precise and approximately 25 times faster at long propagation times than the commonly adopted pseudospectral method. A comparison with the exact solution of the SPE shows that the multisymplectic integration is stable, robust, and preserves the energy functional (see Figure 8 for an example of application of the multisymplectic scheme).

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2.5 Progress for Parabolic Equations with Nonsmooth Data

Robert Haller-Dintelmann and Joachim Rehberg

Starting with the invention of Laplace that the vibrating string can be modeled mathematically by the equation carrying his name since then, the history of partial differential equations goes back more than 250 years. Until today, partial differential equations form, besides modern stochastics, the most adequate and powerful instrument to provide a mathematical model for nature. This concerns nearly all branches of physics, moreover chemistry and biology. Here, partial differential equations often model a certain process, e.g., heat conduction, which is not easy to measure but relatively simple to calculate—provided one has an adequate theory at hand for the corresponding equations, including suitable numerical procedures. The reader may think, e.g., of a semiconductor melt that is contained in a closed chamber and is heated to a temperature above 1,000 K; see [3]. In this case, among other things, the heat fluctuation is of interest. Alternatively, consider the heating of steel under the influence of an electrical field, which is a typical problem in the hardening of steel. A typical example is the heating of a two-dimensional gear rack by direct current as part of a hardening procedure as shown in Figure 1. Optimizing this process, one aims at a uniform temperature of 800 K in the teeth. Figure 1 shows a detail of the toothwork at time $t = 0.2$ sec as a result of a free optimization without additional constraints on the temperature. Due to the high temperature, the material will melt, which has to be prevented. This accentuates the need for an upper bound for the temperature, mathematically speaking, a pointwise state constraint.

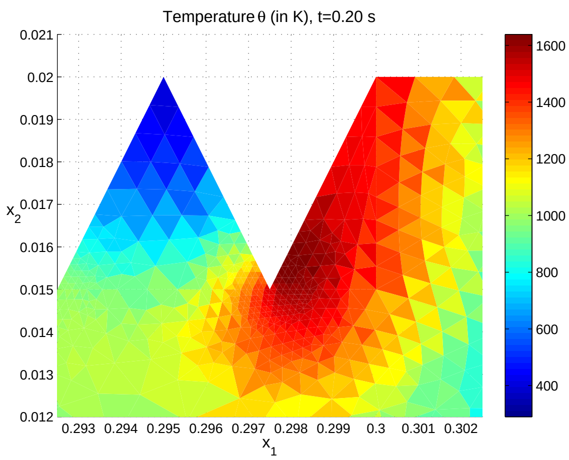

Fig. 1: *Optimal temperature distribution in the teeth of a gear rack*

In both cases, the temperature is described by a nonlinear heat equation. This equation has to be combined with equations determining other physical quantities of interest that enter as parameters in the heat equation. In the case of crystal growth, this is the melt convection, and in the case of steel hardening, it is the occurring electrical field. Within WIAS, such models are investigated in order to improve, together with physicists, the understanding of the physico-chemical processes behind those models and to optimize the procedural methods and instruments.

A large part of second-order partial differential equations may be divided into the classes of elliptic or hyperbolic or parabolic equations, for which the operators

$$\alpha\frac{\partial^2}{\partial x^2}+\beta\frac{\partial^2}{\partial y^2},\quad \alpha\frac{\partial^2}{\partial x^2}-\beta\frac{\partial^2}{\partial y^2},\quad \frac{\partial}{\partial t}-\gamma\frac{\partial^2}{\partial x^2} \tag{1}$$

as the leading terms in the corresponding equations, are prototypes. Besides, the terms *elliptic*, *hyperbolic*, and *parabolic* can be explained as follows: if the operators $\frac{\partial}{\partial x}$ and $\frac{\partial}{\partial y}$ are formally substituted by ξ and η, respectively, then the operators in (1) lead to the polynomials

$$\alpha\xi^2+\beta\eta^2,\quad \alpha\xi^2-\beta\eta^2,\quad \xi-\gamma\eta^2,$$

whose level curves form ellipses, hyperbolas, and parabolas, respectively.

In this article, we deal with parabolic equations, for which the heat equation on a domain Ω

$$u'-\nabla\cdot\rho(u)\mu\nabla u=R(t,u),\quad u(T_0)=u_0, \tag{2}$$

is a prototype. In its simplest form

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

it was already introduced by Fourier in his "Théorie Analytique de Chaleur" (1810–1822). Generically, Ω has a boundary; thus, (2) has to be combined with boundary conditions, which we assume to be mixed in general. This means that on one part Γ of the boundary $\partial\Omega$, Neumann boundary conditions

$$\nu\cdot\rho(u)\nabla u=b_N(t) \tag{3}$$

are prescribed, and on the complement Dirichlet conditions,

$$u|_{\partial\Omega\setminus\Gamma}=b_D(t). \tag{4}$$

Consider, e.g., the example of an iceberg Ω floating partially submerged in water. In this scenario, u is the temperature at the point $x\in\Omega$. On $\partial\Omega\setminus\Gamma$, the portion of $\partial\Omega$ lying below the waterline, Ω behaves like a thermostat; hence, one has to impose a homogeneous Dirichlet boundary condition there. On the remaining portion of the boundary Γ, lying in the air, Ω behaves like a perfect insulator and, thus, one must impose a (homogeneous) Neumann boundary condition on Γ.
Note that, quite analogously, (2) can also be understood as a system. Then u has to be replaced by a vector $\mathbf{u}=(u_1,\dots,u_n)$, and in the j th equation, one has to take $\nabla\cdot\rho(\mathbf{u})\mu\nabla u_j$ instead of $\nabla\cdot\rho(u)\mu\nabla u$. This is quite common in the modeling of reaction-diffusion processes.
Let us first deal with the linear case, which means $\rho\equiv 1$, and $R(t,u)=:f(t)$. Putting $A:=\nabla\cdot\mu\nabla$, equation (2) then reads

$$u'-Au=f,\quad u(T_0)=u_0. \tag{5}$$

Now, one is confronted with the following questions:
Ia) What kind of values is f allowed to take, or, mathematically speaking, what Banach space X is adequate for the solution of (2), (5), respectively?
Ib) What can (must) be assumed on f concerning continuity properties?

II) Is, in particular, either Γ or $\partial\Omega \setminus \Gamma$ empty (pure Dirichlet or pure Neumann case)?
III) What can be imposed on the smoothness of Ω and of the coefficient function μ?

Concerning **I)** and **II)**, there are two principally different situations:
(i) The Neumann condition on Γ is homogeneous, i.e., $b_N(t) \equiv 0$ for every t, and for every t, the value $f(t)$ is a function on Ω.
Then, it is natural to look for a suitable L^p space over Ω and to consider (2) in this space.
(ii) Either the Neumann condition is not homogeneous, or distributional right-hand sides (as, e.g., surface densities or surface recombination) are involved.
In this case, the Banach space X has to be chosen such that—at least—measures on Lipschitz hypersurfaces are contained in X, which, additionally, satisfy a mild regularity assumption. Candidates for X are then Sobolev and Besov spaces, e.g., spaces of type $X = H^{-\theta,q}$, $\theta \in]0,1]$, and $q > 2$ suitably chosen.
If Ω and μ are smooth and only one kind of boundary condition appears, then it is classical how to obtain the solution of the equation (5). Unfortunately, in real-world applications, this is almost never fulfilled: usually, one is confronted with nonsmooth domains, jumping diffusivity coefficients μ, and/or mixed boundary conditions. Thus, one has to make the attempt to re-establish techniques for the nonsmooth case that apply in the smooth situation.
From the classical theory, one knows that the solution u is established by the variation of constants formula

$$u(t) = e^{tA}u_0 + \int_{T_0}^{t} e^{(t-s)A} f(s)\, ds. \tag{6}$$

Consequently, the ultimate questions concerning the generalization to nonsmooth situations are:
IV) Is it possible to give the exponential e^{tA} a precise meaning on the Banach spaces suggested above?
V) Presuming that the right-hand side f has suitable functional-analytic properties, what can one prove on the mapping that assigns to f the right-hand side of (6)?

In order to make this precise, we need the following

Definition. Let $1 < s < \infty$, let X be a Banach space, and let $]T_0, T[\subset \mathbb{R}$ be a bounded interval. Assume that B is a closed operator in X with dense domain D. We say that B has *maximal parabolic $L^s(]T_0,T[;X)$ regularity* if for any $f \in L^s(]T_0,T[;X)$ there exists a unique function $u \in W^{1,s}(]T_0,T[;X) \cap L^s(]T_0,T[;D)$ satisfying

$$u' + Bu = f, \qquad u(T_0) = 0,$$

where the time derivative is taken in the sense of X-valued distributions on $]T_0, T[$.

One of the great advantages of maximal parabolic regularity is to imply simultaneously an affirmative answer for question **IV)**:

Theorem 1. If B has maximal parabolic regularity on a Banach space X, then for every $t > 0$ the exponential e^{-tB} can be properly defined as a bounded operator on X. Moreover, the mapping $]0,\infty[\ni t \mapsto e^{-tB} \in \mathcal{B}(X)$ is analytic.

Another advantage is that the concept of maximal parabolic regularity allows for discontinuous

right-hand sides of the parabolic equations. In particular, the explicit dependence of the reaction term R may be discontinuous. This is important in many examples, in particular, in the control theory of parabolic equations. Alternatively, the reader should think, e.g., of the hardening process of a dental glue, induced by a photoinitiator, where light is switched on/off at a sharp time point and, of course, parameters in the chemical process then change abruptly. It is remarkable that, nevertheless, the solution is Hölder continuous simultaneously in space and time.
The problem, however, consists in the following: despite the fact that the notion of maximal parabolic regularity is well investigated under Banach space aspects, the class of Banach spaces on which divergence operators with nonsmooth coefficients or/and mixed boundary conditions are known to satisfy maximal parabolic regularity was rather poor up to now: it only included Hilbert spaces and L^p spaces. The result on L^p spaces is as follows:

Theorem 2. Assume that Ω is a Lipschitz domain. Let Γ be any open subset of the boundary $\partial\Omega$ and μ be a coeffcient function, which is bounded, elliptic, and takes its values in the set of real, symmetric matrices. Then the operator $-\nabla \cdot \mu\nabla$, complemented with a homogeneous boundary condition on Γ, satisfies maximal parabolic regularity on every space $L^p(\Omega)$ if $p \in]1, \infty[$.

The proof of this theorem heavily rests on so-called *upper Gaussian estimates* and is given in this generality in [5]. This allows for an adequate treatment of (5) in case **(i)**.

In order to treat the case **(ii)**, one has to answer the question whether the operator $-A$ satisfies maximal parabolic regularity on Sobolev/Besov spaces with negative differential index. In the following, we give the answer. For simplicity, we restrict ourselves to the case of three space dimensions, which obviously is the most relevant for applications. Let us first introduce some conventions: by K we denote the unit cube, centered at $0 \in \mathbb{R}^3$, by K_- its lower half, by Σ the upper plate of K_-, and by Σ_0 one half of Σ.

Assumption. For any point $\mathrm{x} \in \partial\Omega$, there is an open neighborhood Υ_x of x and a bi-Lipschitz mapping ϕ_x from Υ_x into $\mathbb{R}^d$, such that $\phi_\mathrm{x}(\mathrm{x}) = 0$, $\phi_\mathrm{x}\big((\Omega \cup \Gamma) \cap \Upsilon_\mathrm{x}\big) = \alpha K_-$ or $\alpha(K_- \cup \Sigma)$ or $\alpha(K_- \cup \Sigma_0)$, for some positive $\alpha = \alpha(\mathrm{x})$. Each mapping ϕ_x is, in addition, volume preserving.

Theorem 3. Assume that $\Omega \cup \Gamma$ satisfies the above assumption and that μ is as in **Theorem 2.** Then $-\nabla \cdot \mu\nabla$ satisfies maximal parabolic regularity on the spaces $H_\Gamma^{-1,q}$ if $q \in [2, 6]$.

Corollary 4. Under the assumptions of **Theorem 3**, $-\nabla \cdot \mu\nabla$ satisfies maximal parabolic regularity also on the real and complex interpolation spaces $(L^p, H_\Gamma^{-1,q})_{\theta,s}$ and $[L^p, H_\Gamma^{-1,q}]_\theta$, where $p \in]1, \infty[$, $q \in [2, 6]$, $\theta \in]0, 1[$, and $s \in]1, \infty[$.

Theorem 3 and **Corollary 4** are proved in [4]. The proof rests heavily on deep results from [1], [2], and localization techniques introduced by Gröger.

Having this at hand, existence and uniqueness for the nonlinear equation (2) may be deduced from a result by Prüss [6], provided one knows that

$$-\nabla \cdot \mu\nabla : H_\Gamma^{1,q}(\Omega) \mapsto H_\Gamma^{-1,q}(\Omega)$$

is a topological isomorphism for a $q > 3$. It was shown at WIAS during the last years that this really holds for nonsmooth situations, including mixed boundary conditions.

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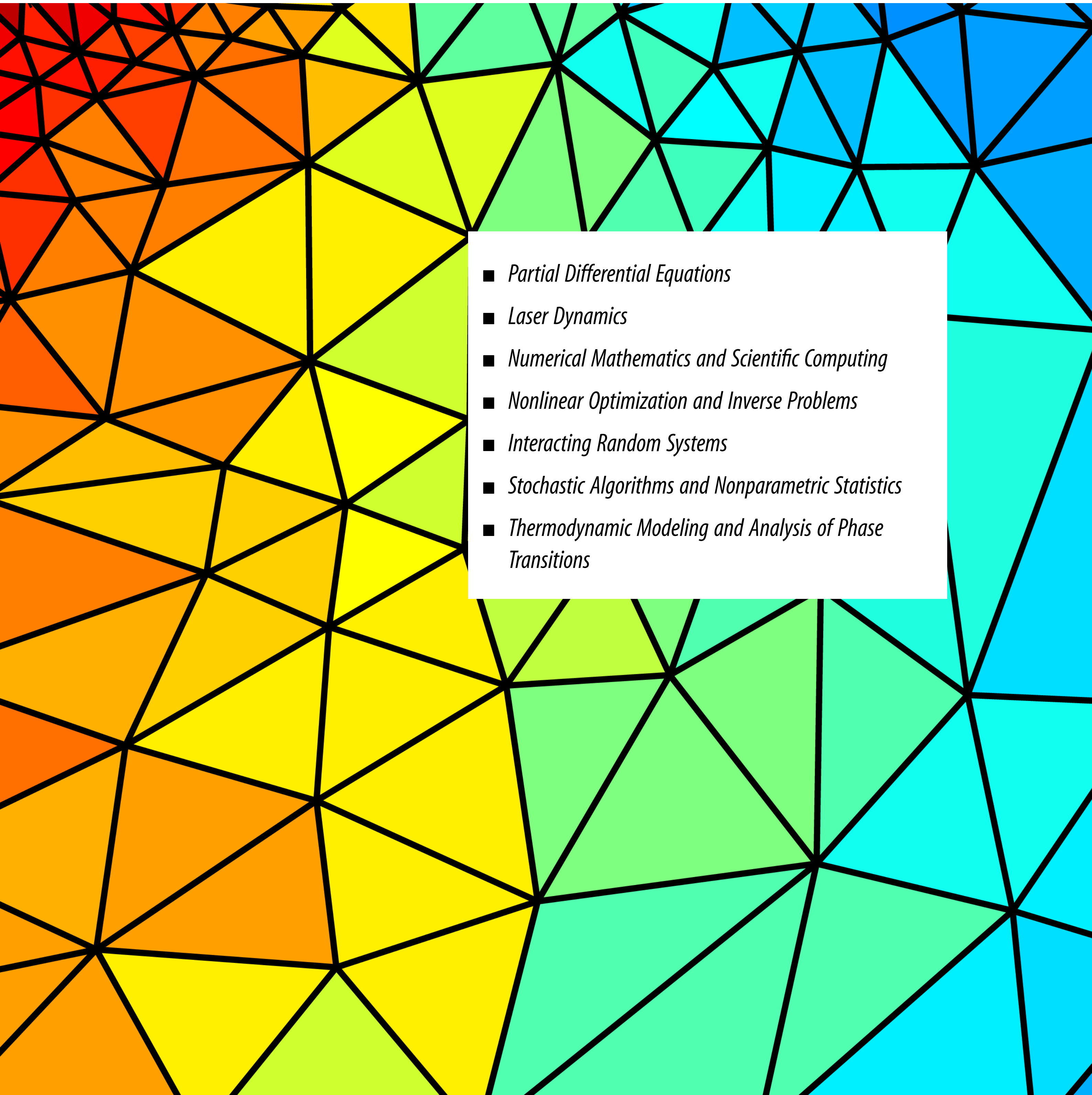
3 Research Groups' Essentials



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

3.1 Research Group *Partial Differential Equations*

The main focus of this research group is the analytical understanding of partial differential equations. The theory is developed in close connection to well-chosen problems in applications, mainly in the following areas:

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

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
- Multiscale methods for the derivation of effective models on larger scales from models on smaller scales

The study of the well-posedness of the underlying partial differential equations leads to a deeper understanding of the underlying physics and provides basic information for the construction of efficient numerical algorithms. In cooperation with other research groups, corresponding software tools are under development that will enable parameter studies or the optimization of technological products.

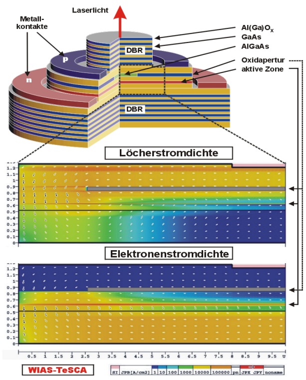


Fig. 1: *Simulation of a VCSEL device using* `WIAS-TeSCA`

In 2007 our group, jointly with research groups *Laser Dynamics* (Uwe Bandelow) and *Numerical Mathematics and Scientific Computing* (Klaus Gärtner), contributed to the proposal of the Collaborative Research Center (SFB) 787 "Semiconductor Nanophotonics: Materials, Models, Devices", which was finally granted for the years 2008–2011 by the German Research Foundation in mid-November. About 20 research groups from the Technical University of Berlin, the Humboldt University of Berlin, Ferdinand Braun Institute for High Frequency Technology, Zuse Institute Berlin (ZIB), the Technical University of Magdeburg, and WIAS were admitted to start their research in early 2008. This SFB aims at the investigation of photonic devices and laser applications, the latter working up to the green spectral range. The topic of project B4 is "Multidimensional modeling and simulation of VCSEL devices" and involves also partners at ZIB. The aim is to combine the specific expertises of ZIB and WIAS in analysis, modeling, and simulation of Maxwell's equations and electric carriers, respectively. Thus, it is intended to develop and to analyze semiclassical models for 3D-structured VCSEL (vertical cavity surface emitting laser) devices, see Figure 1, to implement these models as numerical algorithms, and to perform device simulations by coupling the corresponding software packages (JCMsuite and `WIAS-TeSCA`).

In this field, considerable progress was achieved in the treatment of spatially two-dimensional electro-reaction-diffusion equations, where Annegret Glitzky and Klaus Gärtner (Research Group *Numerical Mathematics and Scientific Computing*) obtained results on thermodynamic equilibria and proved for solutions to the evolution system the monotone and exponential decay of the free energy to its equilibrium value. Thus, the situation of anisotropic materials and rather general statistical relations is included. The same properties were shown for a time- and space-discretized version of the problem [6].

Concerning quantum mechanical modeling, a surprisingly simple proof was found for the monotonicity of the negative particle density operator, which, additionally, enlarges the class of admissible distribution functions up to all discontinuous ones; see [7].

The BMBF project "Application of a nonlocal phase separation model to optical diagnosis of rheumatic diseases", which was a collaboration with Charité Universitätsmedizin Berlin and the Institute for Medical Physics and Laser Medicine, was ended successfully by providing an implementation of a stand-alone, extendable, and portable program for the segmentation of gray-tone pictures to improve the evaluation of scattered-light images of rheumatic finger joints; see [5].

In the field of modeling of multifunctional materials, the year 2007 started with the "6th GAMM Seminar on Microstructures", held at WIAS from January 12 to 13, 2007.

This meeting was also instrumental in the application for the DFG Research Unit (FOR) 797 "Analysis and computation of microstructure in finite plasticity" that was granted in June 2007 and started in September 2007. It involves mathematical and engineering groups in Berlin, Bochum, Duisburg-Essen, Düsseldorf, Leipzig, Regensburg, and Stuttgart.

MICROPLAST

Fig. 2: *Research Unit 797 (supported by DFG)*

The modeling of multifunctional materials was the central theme of several other workshops co-organized by members of our group. The Mathematical Research Institute in Oberwolfach hosted the "Conference on Analysis and Numerics for Rate-Independent Processes" (February 25 – March 3, 2007) organized by Gianni Dal Maso (Trieste), Gilles Francfort (Paris), Tomáš Roubíček (Prague), and Alexander Mielke. It brought together 45 mathematicians and engineers from all over the world.

Two smaller workshops took place in the Centro di Ricerca Matematica "Ennio De Giorgi" in Pisa, Italy. From October 1 to 7, 2007, the "Conference on Structures of the Mechanics of Complex Bodies" presented introductory series of lectures on the topic by C.M. Casciola (Rome), J. Goddard (San Diego), W.K. Liu (Illinois), P.M. Mariano (Florence), A. Mielke, R. Segev (Israel), J. Slawianowski (Warsaw), and A. Visintin (Trento).

The "Workshop on Rate-Independence, Homogenization and Multiscaling" took place from November 15 to 17, 2007, and was organized by Augusto Visintin (Trento) and Alexander Mielke.

The DFG Research Training Group (GRK) 1128 "Analysis, Numerics, and Optimization of Multiphase Problems" organized an Autumn School on the topic "Analysis of Multiphase Problems", which took place in the Institute of Information Theory and Automation (UTIA) in Prague, October 8–12, 2007.

Fig. 3: *Participants of the Autumn School on Analysis of Multiphase Problems in Prague*

The course consisted of three mini-courses of four hours each:

- Eduard Feireisl (Prague): Mathematical theory of multicomponent reactive flows
- Martin Kružík (Prague): Γ-convergence methods and applications
- Alexander Mielke (Berlin): Γ-convergence for evolutionary problems

Additionally, the whole of Thursday was used for short presentations by the Ph.D. students of the RTG as well as some Ph.D. students from Charles University of Prague.

Research in the area of material modeling was mainly devoted to rate-independent models. The MATHEON project C18 "Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys" developed a model describing temperature-driven phase transformations, for which existence and uniqueness results can be derived; see [3]. Elasto-plastic models with linear hardening were studied in [2], providing global spatial regularity results for the displacements, stresses, and internal variables in the time-incremental setting.

In the modeling of damage evolution, a major success was achieved by allowing for complete damage, which means that the material can completely disintegrate in some regions, and the displacements become meaningless in these regions. Using a purely energetic formulation, the displacement can be eliminated, and a suitable Γ-limit can be taken that provides a model involving only damage, energy, and stresses; see [4]. In the Research Training Group (GRK) 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", a Ph.D. position was newly created, where further aspects of damage are investigated. While the above-mentioned work involves damage occurring distributed over three-dimensional volumes, it is also of interest to study the formation and evolution of cracks. In brittle solids like concrete, this can be described by fracture criteria involving the Griffith criterion. A rigorous mathematical framework for the development of a crack along a prescribed crack path is derived and analyzed in [1]. In particular, the notoriously difficult problem of characterizing the physically meaningful jumps is addressed by a vanishing viscosity approach.

Fig. 4: *Research Training Group 1128 (supported by DFG)*

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3.2 Research Group *Laser Dynamics*

The research of the laser dynamics 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 2007 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. Corresponding to these main topics, the group organized in 2007 two international workshops on:

Fig. 1: *Participants of NUSOD 2007, Newark, Delaware, USA*

1. Nonlinear Effects in Photonic Materials (March 2007) and
2. Nonlinear Dynamics and Semiconductor Lasers (November 2007),

which have been highly acknowledged and stimulated further cooperations in these fields. Another highlight in 2007 was the successful habilitation of Andrei Vladimirov at the St. Petersburg State University. The group has extended their teaching activities by a special lecture at the Humboldt University (HU) of Berlin, in addition to their two traditional research seminars with HU and the Free University of Berlin. Again, Uwe Bandelow was a member of the Program Committee of NUSOD, for its 2007 conference in Newark, USA, where he was also invited for a two-hour short course (SC0702) on nonlinear dynamic effects in semiconductor lasers.

In 2007, the research group started a series of new projects funded under the following grants:

1. DFG Research Center MATHEON "Mathematics for key technologies", project D20 "Pulse shaping in photonic crystal fibers": The project is concerned with the property of photonic crystal fibers (PCF) to generate pulses with special spectral characteristics. The propagation of an optical pulse is investigated using the generalized nonlinear Schrödinger equation with focus on soliton propagation, pulse splitting, and the modulation instability (MI) [1]. The results of this analysis are compared with experimental data obtained by collaboration partners at the University of Rostock. A particular aim of this cooperation is to find an appropriate design of the dispersion profile for a PCF that leads to an optimization of the self-organized supercontinuum generation from a nonlinear fiber resonator. Furthermore, the short pulse equation, its properties and multisymplectic numerical integrators, as well as generalizations (jointly with MATHEON project D14) are investigated.
2. DFG, project "Pulse shaping in hollow-fiber compressors: Simulation and experiment", in cooperation with Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin: The goal of this project is a better understanding of the shaping of ultrashort (femtosecond) laser pulses in filaments. In particular, the experimentally observed temporal self-compression shall be explained theoretically as a consequence of the generation of stable propagating asymptotic pulses.

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

3. B4 "Multi-dimensional modeling and simulation of VCSEL devices" (jointly with Alexander Mielke, Research Group *Partial Differential Equations*, and Frank Schmidt, Zuse Institute Berlin)

4. 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*)

In connection with the upcoming SFB 787, especially the research on *mode-locked lasers* played an important role: regular and chaotic interactions of short optical pulses in mode-locked fiber lasers were analyzed within the framework of the generalized complex Ginzburg–Landau equation. Asymptotic equations governing the evolution of coordinates and phases of interacting pulses were derived and studied analytically and numerically [2]. Furthermore, a numerical analysis of the stability of mode-locked regimes in monolithic quantum dot lasers was performed, taking into account carrier exchange processes between quantum dots and wetting layers. The results of this analysis were compared with experimental data obtained at the Technical University (TU) of Berlin [3].

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

1. **Numerical methods for laser dynamics:** Directly modulated lasers have been further investigated using the research group’s software `LDSL-tool` [4] (see also page 135), with special focus on mode selection, needed for applications. Moreover, a system of algebraic equations and inequalities was derived, which allows finding parameters that provide high sensitivity of distributed feedback (DFB) lasers subject to optical feedback. This sensitivity is required to achieve a photon-photon resonance needed for direct modulation applications at high frequencies [4]. By such a theoretical study, e.g., it could be shown that quarter-wavelength shifted single-mode DFB lasers are not advantageous for the required direct modulation applications.

   A new focus in 2007 was placed on the numerical high-performance simulation of the dynamics of semiconductor lasers with stable vertical waveguiding, which is in effect an extension of the traveling wave equation (TWE) model realized in `LDSL-tool` into higher spatial dimensions. Thereby a good qualitative agreement between simulation and experimental data, obtained by collaboration partners at HU Berlin and the Ferdinand Braun Institute for High Frequency Technology, Berlin, could be achieved.

2. **Dynamics of laser systems with delayed coupling or feedback:** This project is funded by the DFG Collaborative Research Center (SFB) 555 “Complex Nonlinear Processes”. It has been successfully evaluated in 2007 and extended until 2010. In 2007, the destabilization scenario in the chain of coupled oscillators and synchronization phenomena in a three-section semiconductor laser [5] have been investigated.

3. **Pulses in nonlinear optical media:** Formation and properties of localized solitary structures propagating in nonlinear media with a special accent on the behavior of ultrashort optical pulses in fused silica were considered both numerically and theoretically in the project D14 “Nonlocal and nonlinear effects in fiber optics” of the DFG Research Center MATHEON “Mathematics for key technologies”.

4. **Dynamical systems:** In 2006/2007, Mark Lichtner developed theoretical functional analytic foundations for a geometric theory of the dynamics of general semilinear hyperbolic systems of equations in one space dimension. Basic results like a variation of constants formula, the principle of linearized stability, existence of smooth invariant manifolds, and bifurcations of

such equations with respect to real-world applications have been obtained [6].
In the framework of activator-inhibitor systems, e.g., Gray–Scott- and Gierer–Meinhardt-type systems, semi-strong pulse interactions were investigated. First, a classical singular perturbation approach was used for the stationary problem. In this way, a manifold of quasi-stationary N-pulse solutions was determined. Then, in the context of the time-dependent problem, an equation for the leading-order approximation of the slow motion along this manifold could be derived. The approach made it possible to treat different types of boundary conditions, to compute folds of the slow manifold, and to identify symmetry-breaking bifurcations in the manifold of two-pulse solutions; see [7].

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3.3 Research Group *Numerical Mathematics and Scientific Computing*

The mathematical description of a significant number of scientific and technological problems leads to *differential equations* that express the relations between temporal and spatial variations of the state of the corresponding physical system. Typically, these equations cannot be solved in closed form, and numerical methods have to 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, 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 step, one is left with a large system of linear (or nonlinear) equations. This system 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. An important aspect is to study the convergence of these approximate models to the original model with finer subdivision in space. 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 software `BOP` (Block Oriented Process simulation), which is based on a divide-and-conquer method. Currently, the main application field is the simulation of gas turbines. The newly delivered release `BOP2.3`, which can now deal with highly complex process description elements as, e.g., “Multiports”, has become the standard tool for gas turbine process simulation at ALSTOM Power Ltd. It is used both for validation/reliability calculations and for the development of new process models. `BOP2.4` has been developed and will be delivered soon. It comprises especially a new simulation mode for correction curve calculation that speeds up this kind of simulation by more than one order of magnitude and enables a more reliable curve representation as well.

Mesh generation

The group focuses on algorithms for the generation of three-dimensional boundary-conforming Delaunay meshes, which are necessary for the implementation of the Voronoi box based finite volume method. The mesh generator TetGen [9] has been established on the international level, as proven by several license requests and a large number of academic users. In 2005, the group initiated a European workshop series "Tetrahedron" focused on grid generation for numerical computations. The second workshop of this series has been held in October 2007 at INRIA Roquencourt, France; the third one is scheduled for 2010 at the University of Swansea, UK.

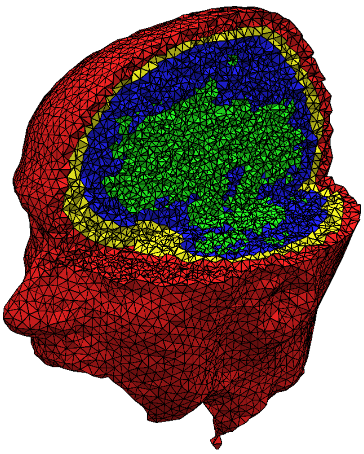

Fig. 1: *Mesh of a human brain generated with TetGen (Geometry: University of Münster)*

Funded by the Dutch research network Ruimte voor Geo-Informatie, in cooperation with the Delft University of Technology (Research Institute OTB, section GISt), the group develops an incremental method for the validation and repair of 3D Piecewise Linear Complexes, which shall be part of an approach to store geometrical objects as, e.g., 3D geodata, using a Constrained Tetrahedralized Irregular Network. Another objective is the use of conforming Delaunay tetrahedralization for efficiently storing objects based on point sets.

Direct solution of large sparse linear systems of equations

In cooperation with Olaf Schenk (University of Basel), the group develops and maintains PARDISO, a sparse direct solver based on the Gauss method tuned in such a way that it runs efficiently on shared-memory parallel computers [8]. This code as well has a large number of academic and commercial uses. It is used in a number of WIAS projects.

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. Current activities include structural improvements of the visualization modules and the addition of vector field visualization.

3D semiconductor device simulation

WIAS's research groups *Partial Differential Equations*, *Laser Dynamics*, and *Numerical Mathematics and Scientific Computing* contributed to the successful institution of the Collaborative Research Center (SFB) 787 "Semiconductor Nanophotonics: Materials, Models, Devices" at the Technical University of Berlin. Figure 2 shows preliminary results of a 3D classical device simulation (the electrostatic potential and the Shockley–Read–Hall recombination distribution) at high injection levels and a typical vertical cavity surface emitting laser (VCSEL) geometry. The challenge is to incorporate the essential effects from the quantum mechanics of quantum dot ensembles to classical heat conduction on the base of mathematical understanding [3] and reliable algorithms [2].

The efficient and accurate solution of eigenvalue problems for Schrödinger operators is essential for the study of quantum mechanical effects in semiconductor devices. Together with our partner Robert Eymard (University Paris-Est), the convergence of the finite volume scheme used to discretize the problem has been proven [6].

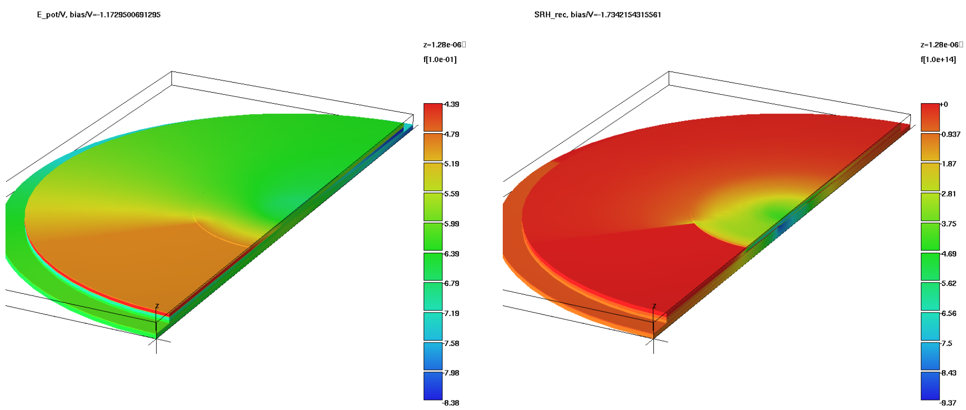

***Fig. 2: Left:** the electrostatic potential distribution in a typical VCSEL geometry with sector-like contacts (red, blue). **Right:** a typical edge singularity defined by the aperture is visible in the Shockley–Read–Hall recombination distribution.*

The longer-term collaboration with Rainer Richter from the Semiconductor Laboratory, Max Planck Institute for Extraterrestrial Physics (HLL), Munich, in silicon detectors shifted slightly from Depleted Field Effect Transistors (DEPFETs) [1] to charge-coupled devices (CCDs). The huge charge clouds (10^7 particles) generated by the future European X-ray laser XFEL raise some general questions for the detector design teams. Efforts have been made to establish a wider collaboration with XFEL-related groups based on results obtained together with HLL Munich. Figure 3 shows results from a study aiming at the improvement of the charge handling capacity of a CCD. Numerically, this means careful computation of charge losses in interacting CCD pixels during charge deposition and charge shifting. 10^6 particles introduce severe nonlinear interactions, while losses of 10 particles in one shift operation are not acceptable. In the actual computations (Figure 3, right), 402,117.39 electrons start in the cloud, 5.785 form the background population at start time, 1.8 electrons are generated by the Shockley–Read–Hall processes during the movement of

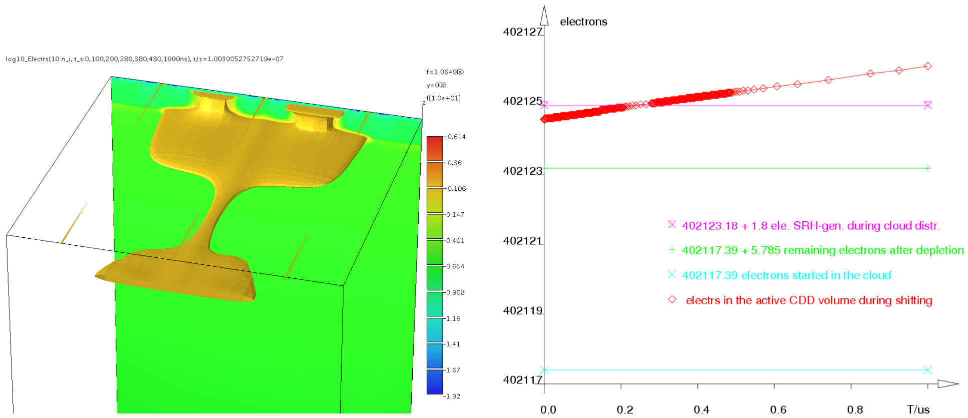

Fig. 3: Left: *electrons are stored in pockets of the electrostatic potential of a CCD and shifted to the next pixel by changing the boundary conditions in time. Parts of eight interacting pixels and the* $10n_i$ *-isosurface of the logarithm of the electron density during shifting are shown.* ***Right:*** *computed electron balance*

the cloud to the potential pockets. During a shift forth and back, the balance is mainly perturbed by Shockley–Read–Hall generation. Less than 0.4 electrons are lost in the active CCD region during this sequence of computations.

Electrochemistry in flow cells and fuel cells

Fuel cells, as possible sources for electrical energy, and thin layer flow cells, used to study electrochemical kinetics, are two types of electrochemical devices where numerical modeling is a base for the deeper understanding of their function. It is specific for flow cells that numerical models are used to support the process of obtaining model parameters.

Funded by the German Ministry of Education and Research in the joint project MikroDMFC (see page 16), the group focused on the numerical modeling of a thin-layer channel flow cell constructed at the University of Ulm (Chair J. Behm). In [4], under a simplifying assumption on the flow, a prototypical numerical method for the identification of kinetic parameters has been presented. Actual results include the successful comparison of the limiting current measurements performed in Ulm with the numerical model [5]. Using the software package COMSOL Multiphysics, the flow regime in coupled fluid systems consisting of free channels and a connected porous so-called *diffusion layer* of a micro direct methanol fuel cell was studied. In cooperation with the Fraunhofer Institute for Reliability and Microintegration (IZM), Berlin, various channel designs have been studied, and a permeability of the porous layer by a fitting procedure has been obtained.

In the framework of the MATHEON project C23 "Mass conservative coupling of fluid flow and species transport in electrochemical flow cells", a successful comparison with experimental results obtained for a cylindrical flow cell at the University of Bonn (Chair H. Baltruschat) has been performed. In this case, the velocity field has been obtained by the numerical solution of the Navier–Stokes equations using finite elements.

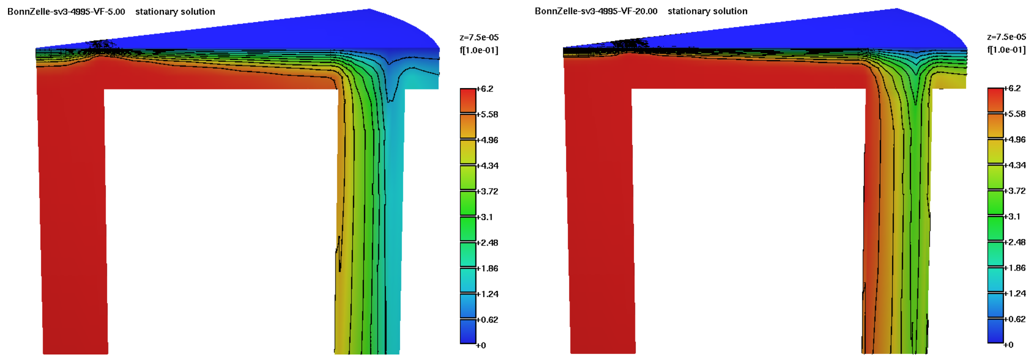

Fig. 4: *Solute concentration in a cylindrical flow cell following the discrete maximum principle at flow rates 5 and 20 $\mu l/s$*

A specific question that arose from this type of applications was the mass conservative coupling between fluid flow and solute transport under preservation of the maximum principle. A successful attempt was the use of the pointwise divergence-free Scott–Vogelius finite element, which has been investigated in detail in [7] (see also the Scientific Highlights article on page 31), together with the Voronoi box based finite volume method and an exact integration of the velocities normal to the finite volume boundaries.

The research under these aspects will be continued within the project “Coupled flow processes in energy and environmental research”, which has been approved by the Senate’s Committee for Competition of the Leibniz Association.

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*: chemical reactions running at an increased temperature transform an acid distribution created by the light into a distribution of a dissolution inhibitor that resists the later applied etching agent. A numerical model for this process step has been developed in cooperation with the group of Andreas Erdmann of the Fraunhofer Institute of Integrated Systems and Device Technology (ISSB) in Erlangen. Continuing this cooperation, we participated in a successful application for an international research network “Material Development for Double exposure and Double patterning” (MD^3) which is funded as a small or medium scale focused research action within the 7th Framework Program of the European Commission. The project focuses on modeling and simulation issues specific to double patterning and double exposure, which are promising modifications of the lithography process aimed at the creation of smaller structures using current exposure technology.

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3.4 Research Group *Nonlinear Optimization and Inverse Problems*

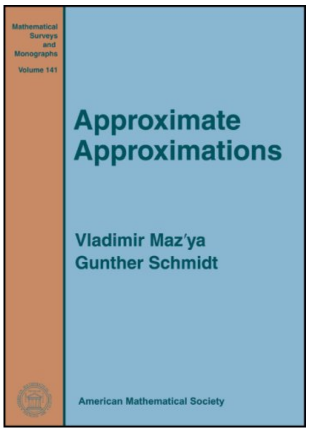
The research group investigates large-scale optimization and inverse problems occurring in current engineering and economic applications. The tasks range from basic research on analysis and numerics to the development of efficient algorithms and software to the solution of real-world problems.

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 82). The group takes part in the Research Training Group 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 TU Berlin and the Scuola Normale Superiore in Pisa.

In 2007, the group has continued its successful cooperation with industry and partners from the engineering sciences. An account of recent results related to scatterometry can be found in the Scientific Highlights article "Mathematical Aspects of Scatterometry – An Optical Metrology Technique" by Andreas Rathsfeld on page 18. It is based on an ongoing research project with Physikalisch-Technische Bundesanstalt (PTB) and is financially supported by the Federal Ministry of Education and Research as part of the project ABBILD.

From a scientific point of view, 2007 was marked by two specific achievements. In cooperation with Masahiro Yamamoto (Tokyo), remarkable progress has been made on uniqueness in inverse acoustic obstacle scattering. In [2], it was proved that a sound-hard polyhedral obstacle in arbitrary dimensions is uniquely determined by its far-field pattern for one incoming plane wave. Together with known results for sound-soft obstacles, this settles completely the uniqueness in the inverse Dirichlet and Neumann problems within the class of polyhedral scatterers.

Secondly, Gunther Schmidt finished his joint monograph with Vladimir Maz'ya (Linköping) [8]. In this book, realizations and applications of a new concept of approximation procedures, called *Approximate Approximations*, are discussed. Most of these procedures, which include approximate quasi-interpolation, interpolation, least-square approximation, cubature of integral operators, and wavelet approximations, have one common feature. They are accurate without being convergent in a rigorous sense. In numerical mathematics, such a situation is not exceptional. For instance, nonconvergent algorithms are well known for solving overdetermined ill-posed problems. The lack of convergence in approximate approximations is compensated for, first of all, by the flexibility in the choice of basis functions and by the simplicity of the multidimensional generalization. Another, and probably the most important, advantage is the possibility to obtain explicit formulas for values of various integral and pseudodifferential operators of mathematical physics applied to the basis functions.



In the sequel, further scientific achievements of the research group in 2007 are detailed.

Optimization and optimal control

The work related to Matheon project C7 "Mean-risk models for electricity portfolio management and stochastic programming" focussed on the theoretical analysis of risk models for stochastic optimization problems in power production. After detailed previous work on models involving risk measures, special attention was paid now to alternative approaches. One of them is based on stochastic dominance constraints. Stability and sensitivity of the corresponding class of optimization problems were investigated in [3]. Another risk-related model analyzed is based on probabilistic constraints. Its study has initiated an intensive cooperation with the research department of Electricité de France (EDF) [4]. This cooperation aims at integrating probabilistic constraints into models for operating hydraulic power units of EDF. A special mathematical challenge here will be the development of suitable dynamic chance constraint models. Finally, a new perspective of this research project has been opened by the analysis of electricity spot markets. In a first step, a characterization of so-called *M-stationary solutions* was provided for a stochastic equilibrium problem under equilibrium constraints (SEPEC) describing a simplified electricity market model.

Regarding the optimal control of PDEs with pointwise state constraints, last year's work on finite element error analysis was carried on. In cooperation with Boris Vexler (RICAM Linz) and Juan Carlos de los Reyes (EPN Quito), the optimal control of the Stokes problem was considered, which required significant extensions of the existing theory; see [7].

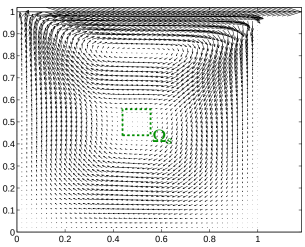


Fig. 1: *Velocity vector field*

Figure 1 shows the result of a state-constrained optimization of a driven cavity flow, i.e., the Stokes problem with homogeneous Dirichlet boundary conditions, except on the upper boundary, where the horizontal velocity takes the value one, while the vertical velocity is zero. The aim was to minimize the L^2 norm of the velocity vector by means of a distributed control, while the Euclidian norm of the velocity must not surpass a given bound in the center of the driven cavity, i.e., in a subdomain $\Omega_s = [7/16, 9/16]^2$. The latter restriction represents a nonlinear pointwise state constraint.

Moreover, the fruitful cooperation with Joachim Rehberg (Research Group *Partial Differential Equations*) on optimality conditions for optimal control problems subject to nonlinear PDE systems and pointwise state constraints was extended. For the state-constrained optimal control of the thermistor problem (see also Figure 1 on page 42), a quasi-linear coupled system of a parabolic and an elliptic PDE, first-order necessary optimality conditions including regular Borel measures as Lagrange multipliers associated with the pointwise state constraints were derived [5]. Together with Robert Haller-Dintelmann (TU Darmstadt), a general class of semilinear elliptic optimal control problems with pointwise state constraints and mixed boundary conditions was investigated. It was possible to prove continuity of the solutions associated with the state equation and to derive necessary and sufficient optimality conditions. A corresponding preprint is in preparation.

Inverse problems

The work with George Hsiao (University of Delaware) on the reconstruction of an elastic body from far field measurements of the acoustic field in a surrounding fluid was continued. The mathematical formulation leads to an inverse transmission problem coupling the Navier system via the obstacle with the Helmholtz equation in the exterior. For its numerical solution, a regularized optimization method was developed, which is based on an analytic formula for the shape derivative of the acoustic field and finite element approximations of the direct problem. Convergence of regularized solutions could be proved, even in the case when the incited elastic wave is not unique, i.e., a Jones mode occurs. Numerical experiments for two-dimensional scatterers confirmed the theoretical results [1].

In connection with a joint project with Wolfgang Bleck, RWTH Aachen, a new view has been taken on the evaluation of dilatometer experiments (cf. Figure 2). Among other things, dilatometers serve to measure the kinetics of solid–solid phase transitions in steel upon cooling from the high temperature phase. Commonly, the data are only used for measuring the start and end temperature of the phase transition. In the case of several coexisting product phases, intricate microscopic investigations have to be performed to obtain the resulting fractions of the different phases. In contrast, it was possible to show that the complete phase transition kinetics including the final phase fractions are uniquely determined by the dilatometer data [6]. Figure 3 depicts a preliminary numerical identification result, proving the feasibility of the new approach.

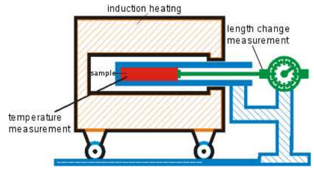


Fig. 2: *Sketch of a dilatometer*

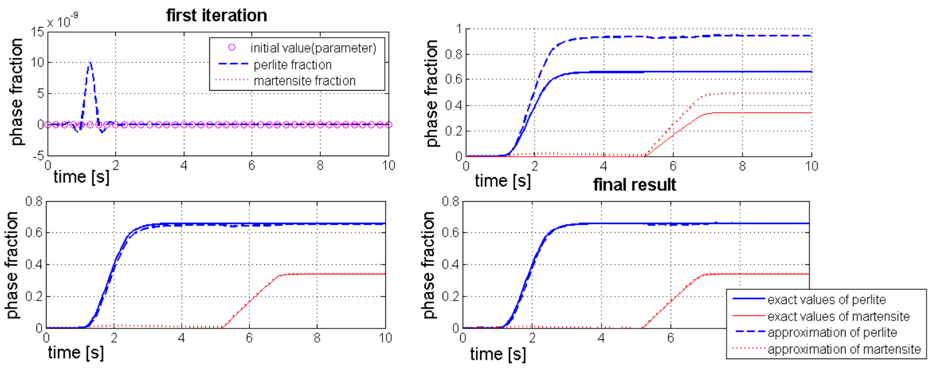


Fig. 3: *Four iterations to identify the phase fraction evolution*

Integral equation methods for diffraction gratings

Grating problems can be treated very efficiently using integral equation methods if the distribution of the optical materials is relatively simple and the interfaces between them are sufficiently regular. Many different, quite sophisticated integral equation formulations for solving the classical diffraction problems have been proposed and implemented. However, a rigorous mathematical and numerical analysis, comparable to standard boundary integral methods, cannot be found in the literature. The preprint [9] contains a study of the mapping properties of boundary integral operators for periodic diffraction as well as the derivation of an integral formulation for the conical diffraction by coated gratings. It generalizes earlier results to the case of oblique incidence and results in a system of four singular integral equations for the nonsmooth grating profiles. It is shown that the integral equations are equivalent to the differential formulation for gratings with non-overhanging profiles or metallic substrate. The strong ellipticity of the integral formulation is established for all relevant physical parameters, which allows to deduce solvability and uniqueness results and the convergence of numerical methods.

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3.5 Research Group *Interacting Random Systems*

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

With the establishment of the DFG International Research Training Group "Stochastic models of complex processes (SMCP)", coordinated by Anton Bovier, in October 2006, the year 2007 was marked by the efforts to get this program off to a good start. One of the highlights here was the first Spring School of SMCP, held at Potsdam University, March 5–9, 2007. Two excellent lecture series by Chris Rogers (Cambridge) and Paolo dai Pra (Padova) were followed by an audience of more than 50 graduate students and postdocs. By now there are 20 graduate students in the Berlin node of SMCP, four of which are supervised at WIAS.

Fig. 1: *Lecture at the Spring School in Potsdam*

Another important event with regard to graduate education was the Summer School on Spin Glasses, held at the University Paris 7 , June 25 – July 6. Anton Bovier was a member of the Scientific Committee and gave two lecture series. Four other members of WIAS participated in the school.

Metastability . . .

Metastability is a ubiquitous phenomenon in nature. It is particularly relevant for the understanding of the onset of dynamical phase transitions where it is often identified with the notion of nucleation. Its mathematical analysis in the context of stochastic dynamics has been a key focus of the research group over the last decade. The so-called *potential theoretic approach* to metastability that was developed here has led to a unified treatment of metastability in many different models and has allowed significant improvements in the precision of estimates of key quantities. A significant drawback up until recently was, however, the fact that good lower bounds on capacities, resp. upper bounds on nucleation times, were not obtainable in situations where the entropy of reaction paths plays a significant rôle. This applies in particular to the key examples of stochastic Ising models at finite (but subcritical) temperatures and/or in infinite volumes.

The last year brought about significant progress in this direction. In a collaboration with Dmitry Ioffe (Haifa), sponsored by a grant from the German-Israeli foundation, a variational principle that expresses the capacity as a supremum over a class of unit flows was implemented to provide sharp lower bounds in the case of the Random Field Curie–Weiss model [1]. This is the first nontrivial model of a spin system where sharp upper and lower bounds for metastable exit times could be derived rigorously.

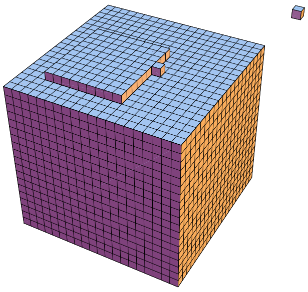

Fig. 2: *Critical droplet for nucleation*

The same variational principle is now also opening doors in other situations, in particular the conservative (Kawasaki) dynamics of the Ising lattice gas, which is being investigated in collaboration with Cristian Spitoni and Frank den Hollander from Eindhoven.

… and ageing

Highly disordered systems, such as spin glasses, provide the canonical examples of so-called *ageing*. In broad terms, a systems is said to age if its time-time correlation functions even at large times do become functions of the time difference only. In other words, an experiment conducted on a sample prepared some time t_w ago can reveal its "age".

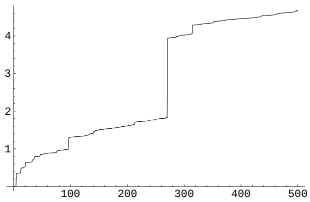

Fig. 3: The α-stable subordinator

Mathematical results concerning ageing in the microscopic dynamics of any interesting systems are extremely scarce. Most of the modeling of ageing systems is done on the level of phenomenological effective models, so-called *trap models*. These are simple Markov chains whose states are intended to represent regions of phase space where the true system is "trapped" for a long time. These trapping times are usually modeled by independent, heavy-tailed (α-stable) random variables. The mathematical analysis of many such trap models has revealed that in most cases the ageing phenomenon is governed by a universal mechanism, the *α-stable Lévy subordinator*.

A considerable breakthrough was achieved in [2] where a similar result could be proven for a large class of microscopic dynamics. Previously, the only example where a connection between spin dynamics and trap models had been established rigorously was the *Random Energy Model*. This could now be widely extended to a large class of Gaussian mean field spin glasses. Moreover, the results apply for a wide range of temperatures and time scales.

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 on different markets and different time scales, also called *stylized facts*. A model to study these mechanisms has been introduced in [3], called *the opinion game*. There, an agent-based model on the level of order-book dynamics is described. Simulations in this model raised questions concerning the stability of markets subject to model parameters involving essentially the behavior of long-term investors.

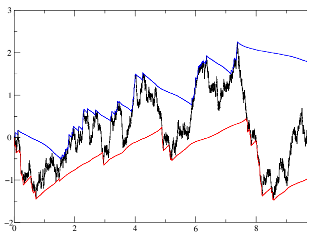

Fig. 4: The three-particle model

These observations motivated the introduction of a simplified model where this question could be studied rigorously. Here, the market is reduced to three particles, representing the current price and the strike prices of long-term investors as buyers resp. sellers. Since long-time investors do not speculate on fast returns, it is reasonable to assume two features: first, the value of the share in the eyes of their holders is much higher than the current price. On the other hand, potential buyers with a long-time horizon will expect to pay less than the current price sometime in the future, because they have the possibility to wait until the price drops. However, both groups of investors will not wait forever. They will modify their opinions in dependence of the price development. The second assumption on the nature of long-time investors, as opposed to short-term traders, is that they will only react slowly to price changes.

The price process is modeled by a stochastic process B, the opinions of buyers $X(B)$ and of sellers $Y(B)$ are described by differential equations with a speed parameter $\gamma > 0$. The larger γ, the smaller the speed of adaptation. It has turned out that γ is a critical parameter for the stability of the model. In particular, for the case that B is a Brownian motion, it was shown that $Y - X$ is recurrent if $\gamma < 1$, and transient if $\gamma > 1$ [9].

As a similar parameter γ also exists in the opinion game, it is possible to draw conclusions on that model. Numerical results show that, depending on γ, the resulting price process can become diffusive if γ is too large (see Figure 5). Our results suggest that this will happen for all $\gamma > 1$, exhibiting a metastable behavior with stable price process on a small timescale and a diffusive one after a phase transition. The three-particle model is an interesting mathematical model in its own right. It will be interesting to investigate the behavior of the system when the price process is not Brownian motion, but, e.g., an α-stable Lévy process.

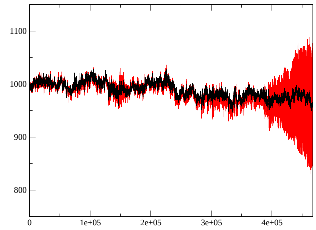

Fig. 5: *The price processes for $\gamma = 1.5$ (black) and $\gamma = 1.6$ (red)*

Stochastic models for spatially extended populations

Stochastic branching models for biological populations, which incorporate "feedback" effects depending on the local population size, are a canonical class of models for ecological systems. One class of models, the so-called *state-dependent branching random walks*, investigated in collaboration with Iljana Zähle (Erlangen), extends the "classical" critically branching random walks where individuals reproduce independently by allowing the rate at which reproductive events occur to be a function of the local occupation number. For this class of models, a functional central limit theorem for the fluctuations of the occupation time of the origin has been obtained in [4]. While these results parallel those known for classical branching random walks, new techniques were required, since the "standard approach", exploiting Laplace transforms, becomes infeasible as soon as dependence is introduced. These techniques, using semimartingale decompositions and stochastic representations for locally size-biased laws, could prove a useful tool for occupation time problems for various interacting particle systems.

In a different line of research, models were considered where, due to competition for resources, the local birth rates are functions of the populations structure, making branching supercritical in sparse regions and subcritical in crowded areas [5]. It has been shown earlier that such systems exhibit unique nontrivial equilibrium. The natural question is then to analyze the space-time mixing properties of this equilibrium and of the behavior of ancestral lineages of individuals sampled from a realization of such an equilibrium. Combined with different types, this research can lead to a microscopic underpinning of Malecot's formula for genetic identity of two individuals sampled at a given distance in a more realistic model with locally randomly fluctuating population densities (as opposed to "classical" population genetic models of the "stepping stone flavor", where population sizes are kept artificially fixed for all time).

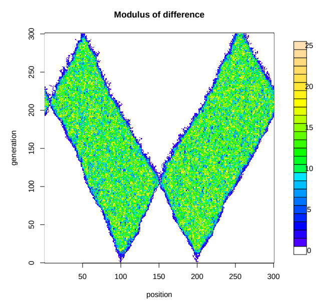

Fig. 6: *Complete convergence for a population system*

Coagulation processes

Further progress has been achieved in the study of stochastic particle models for coagulation processes. Several new results were obtained in collaboration with the Department of Chemical Engineering (University of Cambridge, UK). In [6], the coupling of a stochastic soot algorithm to a deterministic gas-phase chemistry solver was investigated for homogeneous combustion systems.

A particular highlight of the year was the Workshop "Coagulation and Fragmentation Models" in the Mathematical Research Institute in Oberwolfach, organized by Wolgang Wagner together with Jean Bertoin (Paris 6) and James Norris (Cambridge).

Surface growth and fluctuations

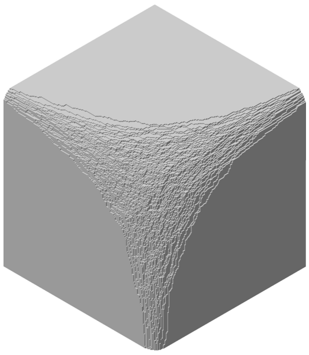

Fig. 7: *3D-Ising corner model: the facet's border is described by the Airy $_2$ process.*

The focus of last year's research in the area of surface growth was on stochastic growth models on a one-dimensional substrate belonging to the KPZ (Kardar–Parisi–Zhang) universality class. The limit process describing the fluctuations of the surface is either the Airy $_2$ or the Airy $_1$ process, depending on whether the limit shape is curved or non-curved. However, there are situations where a curved region and a straight one meet. There, the fluctuations of the surface are described by a transition process, which was discovered in [7]. The work on the Airy $_1$ process was extended in two respects. It was established that this process arises for other models; the polynuclear growth model and discrete-time TASEP with parallel update, and in the so-called *PushASEP* (also called in previous literature "long range exclusion process"). At the same time, these results were extended to "space-like paths". Space-like paths for the asymmetric exclusion process span from tagged particle to fixed-time situations [8].

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3.6 Research Group *Stochastic Algorithms and Nonparametric Statistics*

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

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

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 subprojects A3, A10, and E5 in the DFG Research Center MATHEON, within the project B5 and B9 in the DFG Collaborative Research Center SFB 649 "Economic Risk", and within one project in the DFG Priority Program SPP 1114 "Structure Adaptive Smoothing Procedures with Applications in Imaging and Functional MRI". Members of the group were involved in several industrial contracts. New pricing methods for Bermudan products have led to a continued cooperation with the Landesbank Berlin AG. The problem of pricing and calibration of different financial instruments is the subject of a cooperation with two other banks: Nordbank and Westdeutsche Genossenschafts-Zentralbank.

The group also participates in a contract with ALSTOM (Switzerland) Ltd, Baden, on gas turbine process simulation. The contribution concentrates on general statistical modeling and Monte Carlo approximations.

Scientific highlights achieved by the research group in 2007 are provided below.

Statistical data analysis

Main topics within the project field are *structural adaptive smoothing methods* and methods for *dimension reduction*. The new formal concept of *Propagation and Separation* allows for the selection of critical parameters for the different adaptive procedures developed within this project, i.e., adaptive weights smoothing, stagewise aggregation, and pointwise adaptive procedures, by a common criterion. A monograph is in preparation.

Structural adaptive methods for image denoising are implemented as a package for the R Statistical System that allows to process grey value, color images with colored noise, and mean depending variance.

Our methods for the analysis of functional magnetic resonance experiments have been improved and, in cooperation with partners from Cornell University, shown to be successful in specific applications; see [5].

A first publication on diffusion weighted imaging has been accepted for publication; see [4]. The presentation of these results at the recent Human Brain Mapping Conference has lead to several new contacts in the neuroscience community.

Research on both topics is carried out within the subproject A3 "Image and signal processing in medicine and biosciences" in the DFG Research Center MATHEON.

Recent software developments include a package for the R Statistical System for estimating the effective dimension reduction space in multi-index models.

A novel approach to *dimension reduction*, based on the idea of *Sparse non-Gaussian component analysis* (SNGCA), has been developed in [6]. Within the MATHEON subproject A10, this approach has been successfully applied to modeling the conformation dynamics of real-world stationary molecular systems. The numerical results for medium-sized oligopeptides are reliable even if the conformational changes are rare events on the scale of the complete time series or if the dimension of the state space increases up to 84 in case of B-DNA.

Research within project B5 of SFB 649 focuses on effective dimension reduction for high-dimensional financial data and nonstationary financial and economic time series.

Applied mathematical finance and stochastic simulation

The central theme of this project is the quantitative treatment of problems raised by the industry, based on innovative methods and algorithms developed in accordance with fundamental stochastic principles. The project concentrates on two main areas: *applications in financial industry* and *computational physics*.

The new regression procedure for computing Bermudan upper bounds via linear Monte Carlo, developed in 2006, was further improved. In particular, a systematic approach for setting up a "good" system of basis functions based on hedge controls was discovered [1]. In [3], regression- and consumption-based approaches were allied for the efficient pricing and hedging of callable exotic derivatives (such as snowballs, range accruals, chooser caps). Thus, efficient (non-nested Monte Carlo) procedures for upper bounds of complex structured Bermudan products are obtained. Regression methods have been used for computing option sensitivities (*Greeks*). Combining pathwise methods and difference methods for Greeks with a regression-based approach has led to fast algorithms for sensitivities at an arbitrary state. Furthermore, new probabilistic representations involving approximations of transition densities have been developed in [2] and successfully applied to high-dimensional interest rate products. In the area of (Libor) interest rate modeling, a multivariate stochastic volatility extension of the Libor market model is developed, implemented, and tested. It is shown that the extension allows for flexible, systematic, and robust calibration to market quotes of "caps" and "swaptions", incorporating volatility "smile" and "skew" behavior. Particularly, the new stochastic volatility Libor model and the new efficient algorithms for pricing and hedging of exotic products have attracted the attention of several banks and resulted in intensive collaborations. On the more theoretical side, a breakthrough has been achieved in the study of affine jump processes: for the characteristic function of a general multidimensional affine jump process, different functional series representations are derived. These representations only require explicit knowledge of the (affine) generator and are therefore promising for financial applications. Moreover, the analysis developed in this context allows for an extension to more general process transforms and more general generators and will be the subject of further study.

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

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 arises due to various strong couplings, for example: interface motion produces mechanical stresses; changing electromagnetic fields influence flow patterns; chemical reactions and the appearance of precipitates in crystals lead to lattice deformations; nonlocal radiation fields interact with non-convective heat conduction; long-range interatomic interactions lead to nonlocal PDEs.

New perspectives

There is an increasing industrial demand for optimal design of energy-storing and -converting devices. For this reason, Wolfgang Dreyer and Jürgen Sprekels started two new topics within the research group.

Modeling, analysis, and simulation of the growth process of single crystals with rectangular shape, which are especially needed in photo-voltaic cells: in collaboration with external partners, the analysis and numerics of the related three-dimensional magneto-hydrodynamic system, which moreover is coupled to nonlocal heat conduction, now will become an intensified issue.

The efficiency to convert chemical into electrical energy and the capacity of lithium-ion batteries to store that energy sensitively depend on the functionality of the cathode. Jointly with Miran Gaberščček and Janez Jamnik from the Laboratory for Materials Electrochemistry of the National Institute of Chemistry, Ljubljana, Slovenia, Wolfgang Dreyer developed a new model to describe the processes occurring within the cathode. Its analysis and physical exploitation will become a major topic within the research group in this and the following years; see also the corresponding Scientific Highlights article "The Storage Problem of Rechargeable Lithium-Ion Batteries" by Wolfgang Dreyer on page 24.

Christiane Kraus, jointly with Dorothee Knees (RG 1), successfully submitted a proposal in the framework of the competition "Pakt für Forschung und Innovation" of the German Leibniz Association. The objective of this proposal is to create the new research topic "Mathematical models for failure and fracture mechanics" that will be studied under their supervison within a new subgroup.

Funded projects with industry collaboration

1. The coupling of the transport of heat and matter with time-dependent magnetic fields is treated within the interdisciplinary project KRIST$\widetilde{MAG}$, which is funded by the Zukunftsfonds Berlin. The objective of two industrial companies, physicists, engineers, and mathematicians is the design of a heater-magnet module to control the melt flow and the shape of the melt/crystal interface during crystal growth. The contribution of Wolfgang Dreyer, Pierre-Etienne Druet, Olaf Klein, Christiane Lechner, and Jürgen Sprekels concerns numerical simulations of the growth device as well as analytical investigations of the underlying coupled system of Navier–Stokes equations, the heat equation including radiation, and reduced Maxwell equations.

The in-house code WIAS-HiTNIHS, which has been tremendously improved by Peter Philip within the MATHEON subproject C9 "Numerical simulation and control of sublimation growth of semiconductor bulk single crystals", calculates temperature, heat sources, electric currents, magnetic fields, LORENTZ force, and power supply of the electric coils. The code Navier calculates flow fields in the melt, using the temperature as initial and boundary data and the LORENTZ force as an external force, calculated by WIAS-HiTNIHS. It has become necessary to take care of the three-dimensional structure of the flow pattern in the melt [5]. For small net weight of the melt, the 3D version of Navier, including the mesh generation with the software package TetGen, successfully passed the first tests. We acknowledge the support that was provided by the Research Group *Numerical Mathematics and Scientific Computing* and Eberhard Bänsch from the University of Erlangen.

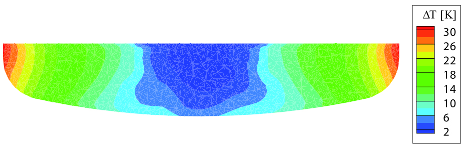


Fig. 1: *3D simulation for small charge size. Temperature distribution at fixed time within the melt. Crystal and crucible are counterrotating at moderate rotation rates.*

Moreover, methods from functional analysis are used to study the stationary as well as the time-dependent solutions of the coupled nonlinear system: Navier–Stokes equations in the Boussinesq approximation, Maxwell equations, heat conduction with convection and radiation. Existence of weak solutions can be guaranteed, estimates on continuous dependence of data, e.g., rotation of the crucible and external electric power, are given. The existent mathematical theory on heat conduction with nonlocal data and on the magneto-hydrodynamical system in nonsmooth domains was improved in a nontrivial manner.

2. Barbara Wagner and Ernst Höschele, in collaboration with Andreas Münch from the University of Nottingham, started a new industrially funded project. A device is considered that consists of an initially plane elastic substrate, covered by a non-Newtonian liquid, set into motion by a rotating cylindrical reel, that is very near to the substrate so that the liquid within the gap forms a thin film. Among the objectives of this study is to find conditions so that the flux of liquid matter through the gap becomes maximal. However, only in the vicinity of the smallest distance between the reel and the substrate, the thin film approximation of the evolution equation for non-Newtonian liquids, i.e., the lubrication approximation, is appropriate. Thus, this simplification cannot be used in the whole domain under consideration. A further complication arises because the elastic substrate behaves

according to the Neo–Hooke elastic law, which is nonlinear with respect to displacement gradients. Finally, it is noted that the surface of the substrate deforms, leading to a free boundary problem. All this leads to a problem of extreme numerical complexity. Currently, the liquid is discarded, and a numerical tool is established that describes the dry contact problem between the cylindrical reel and the Neo–Hooke substrate. Figure 2 indicates for given external load the shape of the free interface and the pressure distribution in the substrate.

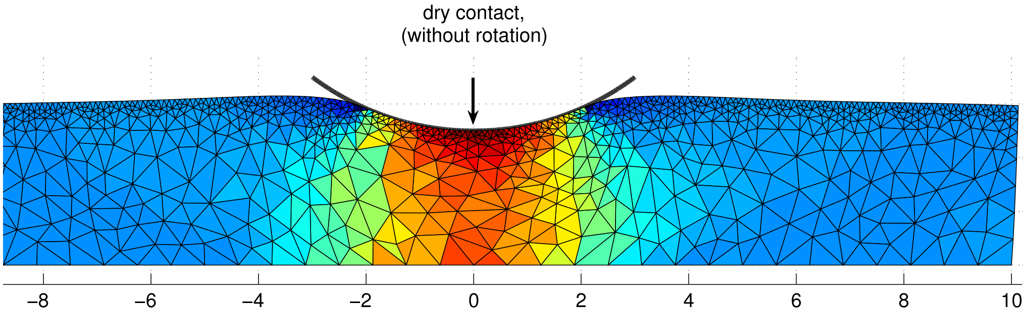


Fig. 2: *Contact problem of a cylindrical reel with a nonlinear elastic substrate. The colors indicate the pressure distribution.*

3. Jointly with an industrial producer of semi-insulating GaAs wafers, the modeling, simulation, and analysis of the dissolution of unwanted precipitates that appear during heat treatment in gallium arsenide (GaAs) wafers has been continued; see [3]. Work on this topic is also funded through two positions within the MATHEON subproject C14 "Macroscopic models for precipitation in crystalline solids", which is headed by Wolfgang Dreyer and Barbara Niethammer from the Mathematical Department of the University of Oxford. Two regimes are alternatively considered to describe the nucleation and subsequent evolution of liquid precipitates in a crystalline matrix. Margarita Naldzhieva studies the first regime where infinite bulk diffusivity in the crystal is assumed and the droplet evolution is modeled by an initial value problem for an ODE system of Becker–Döring type. In the second regime, which is treated by Sven-Joachim Kimmerle, free boundary problems in the crystalline vicinity of each droplet are solved. These lead to a system of many coupled parabolic diffusion equations with local Stefan and Gibbs–Thomson conditions along the droplet/crystal interfaces. The current main objective is the derivation of an effective mean-field PDE that results from homogenization of the many-droplet system.

Funded under Priority Programs of the German Research Foundation

1. Within the Priority Program SPP 1164, Barbara Wagner and Konstantin Afanasiev, in collaboration with Andreas Münch and John King from the School of Mathematical Sciences, University of Nottingham, address the problem of "Mathematical modeling, analysis numerical simulation of thin films and droplets on rigid an viscoelastic substrates, emphasizing the role of slippage". A hierarchy of PDE and ODE models to simulate the evolution of droplets on rigid substrates was developed and tested by a new remeshing algorithm that allows to simulate flow problems in strongly deformable domains with free boundaries. The algorithm now is implemented in the code Navier. Meanwhile, the study on thin films of non-Newtonian liquids in a PET reactor, funded by an individual grant by the German Research Foundation, has been completed; see [1].

2. Funded by the Priority Program SPP 1095, Wolfgang Dreyer and Antonio Segatti continued research on the transition of discrete lattice models described by a large ODE system to a few effective PDEs. More details are to be found in the Scientific Highlights article of the Annual Research Report 2006 "Large Continuum Description of Discrete Lattice Models" by Wolfgang Dreyer and Alexander Mielke, pages 18–26.

Extended Cahn–Hilliard models in four applications

There are four different interdisciplinary applications in the research group where extended Cahn–Hilliard equations are involved.

1. 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, Maciek Korzec, Pete Evans, and Barbara Wagner, jointly with Andreas Münch, School of Mathematics, University of Nottingham, model the epitaxic growth of quantum dots by an extended Cahn–Hilliard equation of spatial order six for the profile of the structure. That equation is a dimension-reduced variation of the elasticity equations similar to the relation between lubrication and Navier–Stokes equations. The mathematical treatment focuses on stationary solutions that were obtained by a new version of formal matched asymptotics that allows to take care of exponentially small terms; see [4].

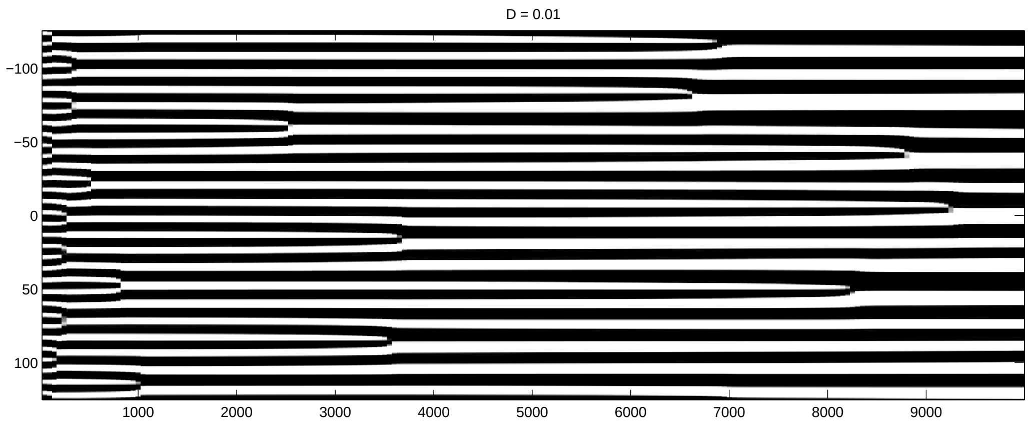


Fig. 3: *Evolution of quantum dots in one space dimension. Left: simplified morphology: triangles on a one-dimensional substrate. Right: slopes* $h_x(t,x)$ *indicated by black and white color versus time*

2. The MATHEON subproject C17 "Adaptive multigrid methods for local and nonlocal phase-field models of solder alloys" is a collaboration with the scientific computing group of Ralf Kornhuber, Free University of Berlin. The project focuses on the numerical treatment of a coupled system consisting of a diffusion equation of Cahn–Hilliard type and the elliptic PDE system for anisotropic elasticity with eigenstrains. That system is currently of enormous importance to model the evolution of lead-free solder joints under extreme thermo-mechanical loads in microelectronic devices. It was modeled by Wolfgang Dreyer in collaboration with Wolfgang Müller, Chair for Continuum Mechanics and Materials Research, Technical University of Berlin; see [2].

3. The analysis of the Cahn–Hilliard equation with mechanical coupling is of extreme complexity. A Ph.D. student of the Research Training Group (GRK) 1128 "Analysis, Numerics, and Optimiza-

tion of Multiphase Problems" studies existence and regularity of solutions, and Christiane Kraus rigorously investigates various sharp-interface limits of the system. Under natural assumptions, existence of minimizers of the corresponding free energy function can be established. To this end, Γ-convergence techniques and geometric measure theory are used.

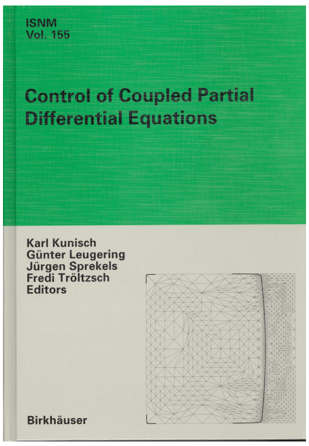
4. The so-called *hyperbolic relaxation of the Cahn–Hilliard equation* adds a second-order time derivative to its classical version. It has important applications if the inertia of the diffusive motion becomes relevant. Antonio Segatti, in collaboration with Riccarda Rossi and Ulisse Stefanelli from the analysis group of the University of Pavia, studies the long-time behavior of this and other dissipative PDEs. In particular, weak solutions are established, and the existence of a unique global attractor can be guaranteed by John Ball's method of semiflows [6].

Ph.D. students

In the context of the various topics of the research group, Wolfgang Dreyer, Jürgen Sprekels, and Barbara Wagner, jointly with other partners, guide and supervise 13 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 and the Humboldt University of Berlin. With respect to the year 2006, the themes have not changed and, therefore, the reader is referred to the Annual Research Report 2006 (pages 74–75) to find precise information on the various objectives, participating institutions, and supervisors.

Miscellaneous

Wolfgang Dreyer and Jürgen Sprekels, jointly with Barbara Niethammer (Mathematical Department, University of Oxford), organized the Workshop "Multiscale Problems in Three Applications" at the Weierstrass Institute, which was funded by WIAS, the DFG Priority Program SPP 1095, and the DFG Research Center MATHEON, see also page 86.



Jürgen Sprekels, jointly with Karl Kunisch (Graz), Günter Leugering (Erlangen), and Fredy Tröltzsch (Technical University of Berlin), organized a Workshop on "Optimal Control of Coupled Systems of PDE" in April 2005 at the Mathematical Research Institute in Oberwolfach. The organizers published the results of that workshop as editors in "Control of Coupled Partial Differential Equations" in the Internat. Series Numer. Math., Vol. 155, Birkhäuser Verlag, Berlin 2007.

Jürgen Sprekels was co-organizer of the "International Conference on Free Boundary Problems" in Chiba, Japan.

As a member of the official delegation of the Federal Minister for Education and Research of Germany, Dr. Annette Schavan, Jürgen Sprekels was speaker at the meeting "Science and Technology in Society" in Kyoto, Japan, in October 2007.

Olaf Klein, jointly with Christiane Frank-Rotsch, Peter Rudolph, Ralph-Peter Lange from the Institute for Crystal Growth, Berlin, and Bernhard Nacke, Technical University of Hannover, applied for a patent on “A new configuration for optimized crystal growth”, EM07-IKZ2.

Wolfgang Dreyer and Frank Duderstadt participate in the initiative “Materials Research for Innovations in the Region of Berlin–Brandenburg” that was started by Brandenburg’s Minister of Science, Prof. Wanka, last September at the University of Potsdam. Its objective is to establish a network between scientific research institutions, i.e., from polymer research, biological medicine, crystal growth, materials science, and small industrial companies and other applicants.

References

[1] K. Afanasiev, A. Münch, B. Wagner, *On the Landau–Levich problem for non-Newtonian liquids*, Physical Review E, **76** (2007), 036307/1–036307/12.

[2] T. Böhme, W. Dreyer, F. Duderstadt, W.H. Müller, *A higher gradient theory of mixtures for multi-component materials*, WIAS Preprint no. 1286, 2007, submitted.

[3] W. Dreyer, F. Duderstadt, *On the modelling of semi-insulating GaAs including surface tension and bulk stresses*, WIAS Preprint no. 995, 2004, to appear in: Proc. R. Soc. A.

[4] M.D. Korzec, P.L. Evans, A. Münch, B. Wagner, *Stationary solutions of driven fourth- and sixth-order Cahn–Hilliard-type equations*, WIAS Preprint no. 1279, 2007, submitted.

[5] C. Lechner, O. Klein, P.-E. Druet, *Development of a software for the numerical simulation of VCz growth under the influence of a traveling magnetic field*, J. Crystal Growth, **303** (2007), pp. 161–164.

[6] R. Rossi, A. Segatti, U. Stefanelli, *Attractors for gradient flows of non-convex functionals and applications*, Arch. Ration. Mech. Anal., **187** (2007), pp. 91–135.

A Facts and Figures

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

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

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

A.1.1 Calls

1. D. Belomestny, Junior professorship, March 5, Humboldt-Universität zu Berlin.

A.1.2 Awards and Distinctions

1. A. Mielke, *member of the council of the International Society for Interaction of Mathematics and Mechanics (ISIMM)*.
2. J. Sprekels, *Chairman of the Board of Forschungsverbund Berlin e.V.*
3. ———, *coordinator of the International Mathematical Science Institutes (IMSI)*.
4. ———, *member of the International Scientific Board of the Institute of Mathematics "Simion Stoilow" of the Romanian Academy, Bucharest*.

A.1.3 Habilitations

1. P. Gapeev, *Optimal stopping problems in mathematical statistics and finance*, Humboldt-Universität zu Berlin, Institut für Mathematik, December 14.
2. A.G. Vladimirov, *Nonlinear dynamics in multimode and spatially extended laser systems*, St. Petersburg State University, Faculty of Physics, June 8.

A.1.4 Ph.D. Theses

1. L.-P. Arguin, *The structure of correlations in quasi-stationary competing particle systems*, Princeton University, Department of Mathematics, November 10.
2. A. Bianchi, *Mixing time for Glauber dynamics beyond* Z^d , Università degli Studi Roma Tre, Department of Mathematics, April 18.
3. M.H. Farshbaf Shaker, *On a nonlocal viscous phase separation problem*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, July 4.
4. A. Linke, *Divergence-free mixed finite elements for the Navier–Stokes equation*, Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Angewandte Mathematik, December 18.
5. A. Schliwa, *Elektronische Eigenschaften von Halbleiterquantenpunkten*, Technische Universität Berlin, Institut für Festkörperphysik, April 25.
6. A. Segatti, *Global attractors for some evolution systems without uniqueness*, University of Milano, Department of Mathematics, January 30.

A.2 Grants[1]

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

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

  "Verbundprojekt: Computergestützte Medizin: Anwendung eines nichtlokalen Phasenseparationsmodells zur Bildbewertung in der Rheumadiagnostik – mathematisch numerischer Teil" (Application of a nonlocal phase separation model to optical diagnosis of rheumatic diseases; in RG 1)
- **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)
- "Abbildungsmethodiken für nanoelektronische Bauelemente" (ABBILD – Imaging Methods for Nanoelectronic Components): cooperation with Physikalisch-Technische Bundesanstalt, Braunschweig and Berlin: "Vermessung von Lithographiemasken durch Scatterometrie" (Measurement of lithographic masks based on scatterometry) (in RG 4)

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)

  A10: "Automatic model reduction for complex dynamical systems" (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)

  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)

  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)
- Exzellenzinitiative (German excellence initiative): „Berlin Mathematical School" (in RG 1, RG 5, and RG 7)

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

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

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

B 02 "Analytische und numerische Untersuchungen von raum-zeitlichen Phänomenen bei gekoppelten Halbleiterlasern" (Analytical and numerical investigation on 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" (Structure-adaptive data analysis; in RG 6)

B7: "Kalibrierungs- und Bewertungsfehler im Risikomanagement" (Calibration and estimation error in risk management; in RG 6)

– 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, RG 3, and RG 4)

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

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

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

"Structure adaptive smoothing procedures with applications in imaging and time series" (in RG 6)

– 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 interaction between structure and process)

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

– 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)

- In 2007, WIAS hosted a scientist with a Heisenberg fellowship (in RG 7).
- A part of the WIAS guest program was supported by DFG grants.

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

- two scholarship holders (in RG 1 and RG 5), see page 127

Deutscher Akademischer Austauschdienst (German Academic Exchange Service), Bonn

- one scholarship holder (in RG 6)

International Projects

- **ESF** (European Science Foundation) Programme "Phase transitions and fluctuation phenomena for random dynamics in spatially extended systems (RDSES)" (in RG 5)
- **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)
- **NATO Linkage Grant:** "Stochastic and computational models of transport in porous media" (in RG 6)
- **SFI Research Frontiers program 2006**: "Bifurcations in systems with hysteresis and nonsmooth nonlinearities" (in RG 2)
- A. Bovier, the head of RG 5, is the Coordinator of the International Research Training Group GRK 1339 "Stochastic Models of Complex Systems and their Applications" (DFG/Swiss National Science Foundation).
- The 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".

Verbundprojekt (research network project): KRISTMAG (in RG 7)

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: “Risikostudie für die Kostenentwicklung des SFEL-Projekts” (Risk study of the development of the costs in the SFEL project; in RG 5)
- Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin: “Mathematische Modellierung und Simulation von MOPA-Diodenlasern” (Mathematical modeling and simulation of MOPA diode lasers; in RG 2)
- HSH Nordbank AG, Kiel: “Robuste Kalibrierung des erweiterten Libor-Markt-Modells” (robust calibration of the extended Libor market model; in RG 6)
- 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)
- pro-Beam Anlagen GmbH, Neukirchen: “Simulation des Elektronen-Mehrspotschweißens von Gusseisen” (Simulation of multispot-welding of cast iron; in RG 4)
- Rücker GmbH, Weingarten: “Simulations- und Optimierungsaufgaben bei der virtuellen Fabrikplanung” (Simulation and optimal control tasks in virtual production planning in automotive industry; in RG 4)
- 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. R. Henrion, Editorial Board, International Journal of Management Science and Engineering Management (MSEM), World Academic Press, Liverpool, UK.
5. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
6. P. Krejčí, Editor, Applications of Mathematics, Academy of Sciences of the Czech Republic, Prague.
7. P. Mathé, Editorial Board, Journal of Complexity, Elsevier, Amsterdam, The Netherlands.
8. ———, Editorial Board, Monte Carlo Methods and Applications, VSP, Zeist, The Netherlands.
9. A. Mielke, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
10. ———, Editor-in-Chief, Journal of Nonlinear Science, Springer Science+Business Media, New York, USA.
11. ———, Editor-in-Chief, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
12. ———, Co-Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
13. ———, Editorial Board, Archive for Rational Mechanics and Analysis, Springer-Verlag, Berlin Heidelberg.
14. ———, Editorial Board, European Series in Applied and Industrial Mathematics: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
15. ———, Editorial Board, Mathematical Models and Methods in Applied Sciences, Imperial College Press, London, UK.
16. J. Polzehl, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.
17. ———, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, The Netherlands.
18. K.K. Sabelfeld, Editor, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
19. ———, Senior Editor, Mathematics and Computers in Simulation, Elsevier, Amsterdam, The Netherlands.
20. V. Spokoiny, Editorial Board, Statistics and Decisions, Oldenbourg Wissenschaftsverlag, München.
21. J. Sprekels, Editorial Board, Applications 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

SIXTH GAMM SEMINAR ON MICROSTRUCTURES
Berlin, January 12–13
Organized by: WIAS (RG 1), DFG (SPP 1195 "Analysis, Modeling and Simulation of Multiscale Problems"), University of Duisburg/Essen
Supported by: SPP 1195, WIAS

WIAS hosted the 6th GAMM Seminar on Microstructures, which is held annually by the GAMM Activity Group "Analysis of Microstructures" in different European places. This seminar brought together 43 mathematicians and researchers from theoretical mechanics, including five international guests. All participants share a common interest in the modeling of multifunctional materials, damage, and microstructure development. The topics of the 21 lectures ranged from analysis using homogenization and relaxation to numerical methods, like FE^2 in plasticity, to configurational-force-driven simulations for crack propagation. The conference was organized by Sergio Conti (Universität Duisburg-Essen) and Alexander Mielke (RG 1). After the event, the Activity Group held its annual, internal assembly.

WORKSHOP "NONLINEAR EFFECTS IN PHOTONIC MATERIALS"
Berlin, March 12–14
Organized by: WIAS (RG 2), University of Bath, UK

The workshop focused on mathematical, physical, and technological aspects of nonlinear optical phenomena in various materials and metamaterials as photonic crystals. The main topics included

- nonlinear fiber optics
- ultrashort pulses
- optical solitons in space and time
- nonlinear effects in new materials
- photonic crystals and microresonators

Major attention has been paid to bringing together the experts from different disciplines, including the mathematical and physical background (including experimentalists) as well as technological applications, with a special focus on optical telecommunication technologies. Especially this interdisciplinary approach as well as the scheduling allowing for intense discussions has been highly acknowledged. The workshop has been attended by 34 participants from 11 countries and included 28 invited and contributed talks.

WORKSHOP "MULTISCALE PROBLEMS IN THREE APPLICATIONS"
Berlin, May 29 – June 1
Organized by: WIAS (RG 7), MATHEON Project Group C14 "Macroscopic models for precipitation in crystalline solids", DFG (SPP 1195 "Analysis, Modeling and Simulation of Multiscale Problems"), Humboldt-Universität zu Berlin (HU)
Supported by: DFG Research Center MATHEON, SPP 1195, WIAS

Within the focus of the workshop were three categories of multiscale problems with simultaneous scalings of time, space, and further quantities that are characteristic for the case at hand.

- Discrete lattice models and their continuum limits
- Discrete and continuum descriptions of nucleation and subsequent evolutions
- Sharp interface limits of phase field systems

Discrete lattice models serve as prototypes to study various possible limiting cases where a discrete ODE system can be substituted by a single or at least a few PDEs that describe the discrete dynamics on a continuum level.

During the first stages of a phase transition, small clusters of the new phase with α particles may grow or shrink by adding or subtracting a single particle. The evolution of the number of clusters is described by an ODE system of Becker–Döring type, which, however, should be substituted by a PDE if clusters above a certain size appear.

Phase field systems resolve the interfacial region so that their evolution may be described by smooth fields. On the scale of microscopic observations, the interfacial region mostly appears as a singular surface, where the observable fields change discontinuously. Thus the physical relevance of phase field systems is tested by their sharp interface limits.

The workshop was attended by 46 participants. Twenty talks were given.

WORKSHOP "NONLINEAR DYNAMICS IN SEMICONDUCTOR LASERS"
Berlin, November 19–21
Organized by: WIAS (RG 2), MATHEON Project Group D8 "Nonlinear dynamical effects in integrated optoelectronic structures"
Supported by: DFG Research Center MATHEON

The main focus of the workshop was concentrated on the development of numerical and analytical approaches to study different nonlinear dynamical regimes in semiconductor laser devices and integrated optoelectronic structures. Furthermore, recent results on modeling, analysis, and experimental study of various types of modern optoelectronic devices were presented. Among the topics discussed, the main emphasis was given to semiconductor ring lasers, multi-section mode-locked lasers, high-power tapered lasers, and different modifications of lasers based on novel quantum-dot active media.

The main goal of the workshop was to bring together mathematicians, physicists, and engineers working in the fields of mathematical modeling, analysis, experimental study, and fabrication of semiconductor optoelectronic devices. Forty-nine participants from 9 European countries participated in the workshop. There were 19 invited talks (15 among them were given by scientists from abroad) and 10 contributed presentations, devoted to different theoretical and experimental aspects of semiconductor laser dynamics. The full program of the workshop can be found at the web page `http://www.wias-berlin.de/workshops/NDSL07/`.

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

1. U. BANDELOW, member of the Organization Committee, *7th International Conference "Numerical Simulation of Optoelectronic Devices" (NUSOD'07)*, University of Delaware, Newark, USA, September 23–27.
2. M. BIRKNER, co-organizer of the minisymposium M16 "Stochastic models in population genetics: Coalescents, random trees and application", *Gemeinsame Jahrestagung der Deutschen Mathematiker-Vereinigung und der Gesellschaft für Didaktik der Mathematik 2007*, Humboldt-Universität zu Berlin, March 26–27.
3. A. BOVIER, co-organizer, *Spring School of the International Research Training Group "Stochastic Models of Complex Processes"*, Potsdam, March 5–9.
4. ———, member of the Organizing Committee, *BRG Workshop on Random Spatial Models from Physics and Biology (Dutch-German Research Group)*, Universität Bielefeld, Fakultät für Mathematik, March 30–31.
5. ———, co-organizer, *École d'été "Verres de Spin"*, Institut de Mathématiques de Jussieu, Paris, France, June 25 – July 6.
6. ———, member of the Organizing Committee, *BRG Workshop on Random Spatial Models from Physics and Biology (Dutch-German Research Group)*, EURANDOM, Eindhoven, The Netherlands, November 1–3.
7. R. HENRION, co-organizer, *International Congress "Mathematical Methods in Economics and Industry" (MMEI 2007)*, Herlany, Slovakia, June 3–7.
8. D. HÖMBERG, organizer of the minisymposium "Mathematics for steel manufacturing", *6th International Congress on Industrial and Applied Mathematics (ICIAM 2007)*, ETH Zürich, Switzerland, July 16–20.
9. ———, organizer of the minisymposium "Inverse problems in electromagnetic scattering", *6th International Congress on Industrial and Applied Mathematics (ICIAM 2007)*, ETH Zürich, Switzerland, July 16–20.
10. ———, co-organizer, *Industrial and Interdisciplinary Workshop "Problems Related to the Manufacture of Multiphase Steels"*, University of Oxford, Oxford Centre for Industrial and Applied Mathematics, UK, November 2.
11. H.-CHR. KAISER, co-organizer, *6th Workshop on Multiscale Problems in Quantum Mechanics*, Universität Tübingen, February 8–9.
12. A. MIELKE, co-organizer, *Analysis and Numerics for Rate-Independent Processes*, Mathematisches Forschungsinstitut Oberwolfach, February 25 – March 3.
13. ———, member of the Program Committee, *6th International Congress on Industrial and Applied Mathematics (ICIAM 2007)*, ETH Zürich, Switzerland, July 16–20.
14. ———, member of the Scientific Committee, *International Conference on Differential Equations (EQUADIFF 07)*, Vienna University of Technology, Austria, August 5–11.
15. ———, co-organizer, *Workshop "Structures of the mechanics of complex bodies"*, Centro di Ricerca Matematica "Ennio De Giorgi", Pisa, Italy, October 1–7.
16. ———, co-organizer, *Autumn School "Analysis of Multiphase Problems" of the Research Training Group "Analysis, Numerics, and Optimization of Multiphase Problems" (GRK 1128)*, Nečas Center for Mathematical Modeling and Institute of Information Theory and Automation, Prague, Czech Republic, October 8–12.
17. ———, co-organizer, *Workshop on Rate-Independence, Homogenization and Multiscaling*, Centro di Ricerca Matematica "Ennio De Giorgi", Pisa, Italy, November 15–17.
18. H. NEIDHARDT, chairman of the Section 3a "Operator theory in Hilbert and Krein spaces and applications", *Modern Analysis and Applications – 2007, dedicated to the centenary of Mark Krein*, Odessa National I.I. Mechnikov University, Institute of Mathematics, Economics and Mechanics, Ukraine, April 9–14.
19. ———, chairman of a plenary session, *10th Quantum Mathematics International Conference (QMath 10)*, Romanian Academy, Institute of Mathematics "Simion Stoilow", Moeciu, Romania, September 10–15.
20. K.K. SABELFELD, member of the Program Committee, *VI IMACS Seminar on Monte Carlo Methods (MCM 2007)*, University of Reading, UK, June 18–21.

21. J. Sprekels, co-organizer of the minisymposium “Phase Transitions and Hysteresis in Free Boundary Problems”, *Joint International Meeting UMI-DMV 2007*, Universitá degli Studi di Perugia, Italy, June 18–22.
22. ———, member of the Organizing Committee, *International Conference on Free Boundary Problems (FBP2007) “Nonlinear Phenomena with Energy Dissipation: Mathematical Analysis, Modelling and Simulation”*, Chiba University, Japan, November 26–30.
23. W. Wagner, co-organizer, *Coagulation and Fragmentation Models*, Mathematisches Forschungsinstitut Oberwolfach, September 23–29.

A.6 Publications

A.6.1 Monographs

[1] E. Holzbecher, *Environmental Modeling: Using MATLAB*, Springer, Heidelberg, 2007, xvii+392 pages.

[2] V. Maz'ya, G. Schmidt, *Approximate Approximations*, vol. 141 of Mathematical Surveys and Monographs, American Mathematical Society, Providence, 2007, 349 pages.

A.6.2 Editorship of Proceedings and Collected Editions

[1] E. Bolthausen, A. Bovier, eds., *Spin Glasses*, vol. 1900 of Lect. Notes Math., Springer, Berlin-Heidelberg, 2007, 179 pages.

[2] K. Kunisch, G. Leugering, J. Sprekels, F. Tröltzsch, eds., *Control of Coupled Partial Differential Equations*, vol. 155 of Internat. Series Numer. Math., Birkhäuser, Berlin, 2007, 382 pages.

A.6.3 Articles in Refereed Journals[2]

[1] M. Eleuteri, *Regularity results for a class of obstacle problems*, Appl. Math., 52 (2007), pp. 137–170.

[2] ———, *Well-posedness results for a class of partial differential equations with hysteresis arising in electromagnetism*, Nonlinear Anal. Real World Appl., 8 (2007), pp. 1494–1511.

[3] K. Afanasiev, A. Münch, B. Wagner, *On the Landau–Levich problem for non-Newtonian liquids*, Phys. Rev. E, 76 (2007), pp. 036307/1–036307/12.

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[85] H. Stephan, A. Khrabustovskyi, *Positivity and time behavior of a general linear evolution system, non-local in space and time*, Preprint no. 1264, WIAS, Berlin, 2007.

[86] K. Tabelow, J. Polzehl, V. Spokoiny, H.U. Voss, *Diffusion Tensor Imaging: Structural adaptive smoothing*, Preprint no. 1232, WIAS, Berlin, 2007.

[87] M. Tlidi, A. Mussot, E. Louvergneaux, G. Kozyreff, A. Vladimirov, A. Taki, *Control and removing of modulational instabilities in low dispersion photonic crystal fiber cavities*, Preprint no. 1201, WIAS, Berlin, 2007.

[88] A. Yulin, D. Skryabin, A. Vladimirov, *Modulational instability of discrete solitons in coupled waveguides with group velocity dispersion*, Preprint no. 1198, WIAS, Berlin, 2007.

[89] V. Vatutin, V. Wachtel, *Local limit theorems for ladder moments*, Preprint no. 1200, WIAS, Berlin, 2007.

[90] R. Fetzer, A. Münch, B. Wagner, M. Rauscher, K. Jacobs, *Quantifying hydrodynamic slip: A comprehensive analysis of dewetting profiles*, Preprint no. 1220, WIAS, Berlin, 2007.

[91] J.R. King, A. Münch, B. Wagner, *Linear stability analysis of a sharp-interface model for dewetting thin films*, Preprint no. 1248, WIAS, Berlin, 2007.

[92] M. Wolfrum, J. Ehrt, *Slow motion of quasi-stationary multi-pulse solutions by semistrong interaction in reaction-diffusion systems*, Preprint no. 1233, WIAS, Berlin, 2007.

[93] S. Yanchuk, M. Wolfrum, *Destabilization patterns in large regular networks*, Preprint no. 1213, WIAS, Berlin, 2007.

A.7.2 Preprints/Reports in other Institutions

[1] A. Bradji, R. Herbin, *Discretization of the coupled heat and electrical diffusion problems by the finite element and the finite volume methods*, Preprint no. 6632, Laboratoire d'Analyse, Topologie, Probabilités, Marseille, France, 2007.

[2] P.-E. Druet, *On existence and regularity of solutions for a stationary Navier–Stokes system coupled to an equation for the turbulent kinetic energy*, Tech. Report no. 13, Humboldt-Universität zu Berlin, Institut für Mathematik, 2007.

[3] M.C. Babiuc, S. Husa, I. Hinder, Ch. Lechner, E. Schnetter, B. Szialagyi, Y. Zlochower, N. Dorband, D. Pollney, J. Winicour, *Implementation of standard testbeds for numerical relativity*, arXiv:0709.3559 [gr-qc], Cornell University, Ithaca, NY, USA, 2007.

[4] B. Hofmann, P. Mathé, S.V. Pereverzev, *Regularization by projection: Approximation theoretic aspects and distance functions*, Preprint no. 10, Technische Universität Chemnitz, Fakultät für Mathematik, 2007.

[5] P. Colli, A. Segatti, *Uniform attractors for a phase transition model coupling momentum balance and phase dynamics*, Preprint no. 20PV07/19/0, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche, Pavia, Italy, 2007.

[6] F. Drechsler, C.H. Wolters, T. Dierkes, H. Si, L. Grasedyck, *A highly accurate full subtraction approach for dipole modelling in EEG source analysis using the finite element method*, Preprint no. 95, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, 2007.

A.8 Talks, Posters, and Contributions to Exhibitions

A.8.1 Scientific Talks (Invited)

1. G. Basile, *Kinetic limit for the harmonic chain perturbed by a conservative noise*, Boltzmann 2007, October 16–19, Institut Henri Poincaré (IHP), Paris, France, January 17.
2. A. Münch, *Sharp-interface models & contact line instabilities for dewetting films*, Summer Workshop 2007 of the DFG Priority Program SPP 1164 "Nano- and Microfluidics", August 1–3, Bad Honnef, August 2.
3. O. Zindy, *One-dimensional transient random walks in random environment in the sub-ballistic regime*, Arbeitsgemeinschaft Percolation, October 7–13, Mathematisches Forschungsinstitut Oberwolfach, October 9.
4. ———, *Aging and quenched localization for one-dimensional random walks in random environment in the sub-ballistic regime*, Université Versailles Saint Quentin en Yvelines, France, November 26.
5. S. Amiranashvili, *Turing instability of electrical discharges*, Workshop Selbstorganisation und Komplexität, August 25–31, Westfälische Wilhelms-Universität Münster, Institut für Theoretische Physik, Ameland, Niederlande, August 27.
6. L.-P. Arguin, *The structure of quasi-stationary competing particle systems*, Workshop "Particle systems, non-linear diffusion and equilibration", November 2–30, Universität Bonn, Hausdorff Research Institute for Mathematics, Program "Complex Stochastic Systems: Discrete vs. Continuous", November 12.
7. U. Bandelow, *Nichtlineare Effekte in Halbleiterlasern und optischen Fasern*, Habilitandenkolloquium, Humboldt-Universität zu Berlin, Institut für Physik, April 17.
8. ———, *Efficient modeling and analysis of dynamical effects in semiconductor laser devices*, University of Nottingham, George Green Institute, UK, July 6.
9. ———, *Semiconductor laser instabilities and dynamics (Short Course SC 0702)*, 7th International Conference "Numerical Simulation of Optoelectronic Devices" (NUSOD'07), University of Delaware, Newark, USA, September 25.
10. ———, *Non-Raman redshift by pulse splitting*, 7th International Conference "Numerical Simulation of Optoelectronic Devices" (NUSOD'07), September 24–27, University of Delaware, Newark, USA, September 27.
11. ———, *Enhanced modulation bandwidth by integrated feedback*, Rio de la Plata Workshop on Noise, Chaos and Complexity in Lasers and Nonlinear Optics, December 3–6, Punta del Este, Uruguay, December 5.
12. D. Belomestny, *Fast upper bounds for Bermudan products*, Deka Bank, Frankfurt am Main, January 11.
13. ———, *True upper bounds for Bermudan products via non-nested Monte Carlo*, Frankfurt MathFinance Workshop on Derivatives and risk management in theory and practice, March 26–27, Frankfurt am Main, March 27.
14. ———, *Spectral estimation of the fractional order of a Levy process*, Cemapre Conference on Advances in Semiparametric Methods and Applications, Satellite meeting of ISI 2007, August 20–21, Lisbon, Portugal, August 20.
15. ———, *A jump-diffusion Libor model and its robust calibration*, Mini-Workshop on Calibration, Lévy processes in finance, FFT, and related issues, Technische Universität Wien, Austria, November 16.
16. A. Bianchi, *Mixing time for Glauber dynamics beyond* Z^d, Università degli Studi dell'Aquila, Facoltà di Scienze Matematiche, Fisiche e Naturali, Italy, April 11.
17. ———, *Mixing time for Glauber dynamics beyond* Z^d, Università di Roma Tre, Dipartimento di Matematica, Italy, April 17.
18. M. Birkner, *Variations on the coalescent and fitting real data*, Probability and Statistics in Population Genetics, January 22–26, University of Leiden, Lorentz Center, The Netherlands, January 26.

19. ———, *Likelihood-based inference for Λ-coalescents*, Workshop on Mathematical Modelling and Analysis of Biological Networks, January 29 – February 2, University of Leiden, Lorentz Center, The Netherlands, February 2.
20. ———, *Quenched LDP for words in a letter sequence*, September 17–20, EURANDOM, Eindhoven, The Netherlands, September 18.
21. ———, *Computing likelihoods under Λ coalescents (in the infinitely-many-sites model)*, Workshop "Coagulation and Fragmentation Models", September 23–29, Mathematisches Forschungsinstitut Oberwolfach, September 27.
22. ———, *Conditional LDP for sentences and applications*, BRG Workshop on Random Spatial Models from Physics and Biology, November 1–3, EURANDOM, Eindhoven, The Netherlands, November 2.
23. ———, *Bedingtes großes Abweichungs-Prinzip für Sätze und Anwendungen*, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, November 15.
24. ———, *Conditional LDP for words in a letter sequence*, University of Oxford, Department of Statistics, UK, November 20.
25. ———, *Towards a mathematical population genetics with highly skewed offspring distributions*, Rhein-Main Kolloquium Stochastik, Johann Wolfgang Goethe-Universität Frankfurt am Main und Johannes Gutenberg Universität Mainz, November 28.
26. A. Bovier, *Recent progress on the spin glass problem*, Oxford-Warwick-London (OWL) Meeting "Combinatorics, Probability and Statistical Mechanics", University of Oxford, UK, January 31.
27. ———, *Universality of ageing in mean field spin glasses*, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, March 15.
28. ———, *Universality of ageing in mean field spin glasses*, Universität Zürich, Institut für Mathematik, Switzerland, April 3.
29. ———, *Universality of ageing in mean field spin glasses*, Mathematical Physics Seminar, Princeton University, Department of Mathematics, USA, May 3.
30. ———, *Ageing in spin glasses at intermediate time scales: Universality of the trap model*, 97th Rutgers Conference on Statistical Mechanics, May 6–8, Rutgers University, Mathematics Department, USA, May 8.
31. ———, *Ageing in spin glass models at intermediate time scales: Universality of the trap model*, Workshop "Phase Transitions", June 3–9, Mathematisches Forschungsinstitut Oberwolfach, June 6.
32. ———, *Short course: Introduction to the statistical mechanics of disordered systems*, 4 talks, École d'été Verres de Spin, Institut de Mathématiques de Jussieu, Paris, France, June 25 – July 6.
33. ———, *Short course: Random energy model and spin glasses with tree structure: A rigorous approach*, 4 talks, École d'été Verres de Spin, Institut de Mathématiques de Jussieu, Paris, France, June 25 – July 6.
34. ———, *Ageing in mean field spin glasses*, Workshop "Large Scale Stochastic Dynamics", August 26 – September 1, Mathematisches Forschungsinstitut Oberwolfach, August 29.
35. ———, *Mini-course: Equilibrium and dynamics of spin glasses*, 2 talks, Peking University, China, September 11.
36. ———, *Metastability: A potential theoretic approach*, Mathematics Colloquium, Peking University, China, September 14.
37. ———, *Ageing in mean field spin glasses*, Academia Sinica, Beijing, China, September 17.
38. ———, *Mini-course: Equilibrium and dynamics of spin glasses*, 2 talks, Beijing Normal University, China, September 18.
39. ———, *Metastability*, Chinese University of Mining and Technology, Xuzhou, China, September 24.
40. ———, *Metastability in the random field Curie–Weiss model*, Workshop "Particle systems, nonlinear diffusions, and equilibration", November 12–16, Universität Bonn, Hausdorff Research Institute for Mathematics, Program "Complex Stochastic Systems: Discrete vs. Continuous", November 16.
41. ———, *Lecture series: Long term dynamics of disordered systems: From metastability to ageing*, 6 talks, Universität Bonn, Hausdorff Research Institute for Mathematics, Program "Complex Stochastic Systems: Discrete vs. Continuous", November 20–30.

42. ———, *Metastability in the random field Curie–Weiss model*, Workshop on Dynamical Systems, November 30 – December 2, Universität Bielefeld, Mathematisches Institut, December 1.
43. Y. Chen, *Accounting for nonstationarity and heavy tails in financial time series, with applications to robust risk management*, Financial Mathematics Seminar, University of Chicago, Center for Financial Mathematics, USA, January 19.
44. W. Dreyer, *Evolution of bubbles in a ternary liquid*, Second Workshop "Micro-Macro Modelling and Simulation of Liquid-Vapour Flows", January 10–12, Université Bordeaux I, Institut de Mathématiques and INRIA, France, January 11.
45. ———, *On existence and validity of the maximum entropy principle*, The Sixth Workshop on "Multiscale Problems in Quantum Mechanics and Averaging Techniques", February 8–9, Universität Tübingen, February 9.
46. ———, *Evolution of microstructures in modern materials due to diffusional processes with thermodynamical coupling*, Workshop on Rock Mechanics and Logistics in Mining, February 26 – March 2, Santiago de Chile, March 2.
47. ———, *A study of heat conduction in the vicinity of phase boundaries*, 5. Workshop "Angewandte Simulation in der Kristallzüchtung", April 25–26, Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung e.V. (DGKK), Iphofen, April 26.
48. ———, *Capabilities of phase field models*, Electrochemical Seminar, May 3–4, National Institute of Chemistry, Ljubljana, Slovenia, May 3.
49. ———, *Modeling of nucleation phenomena*, Workshop "Phase Transitions", June 3–9, Mathematisches Forschungsinstitut Oberwolfach, June 5.
50. ———, *Conservation laws and kinetic relations in the context of a rechargeable lithium battery*, 8th Hirschegg Workshop on Conservation Laws, September 9–15, September 13.
51. ———, *Phase transitions and hysteresis in rechargeable lithium batteries*, International Conference on Free Boundary Problems (FBP2007) "Nonlinear Phenomena with Energy Dissipation: Mathematical Analysis, Modelling and Simulation", November 26–30, Chiba University, Japan, November 29.
52. ———, *Hysterese und Phasenübergänge in wiederaufladbaren Lithium-Batterien*, Composite Forschung in der Mechanik, December 3–5, Universität Paderborn, Lehrstuhl für Technische Mechanik, December 4.
53. P.-E. Druet, *Schwache Lösung für ein Modell elektromagnetischen Heizens mit Wärmestrahlung*, Seminar Optimale Steuerung von Partiellen Differentialgleichungen, Technische Universität Berlin, Institut für Mathematik, May 24.
54. F. Duderstadt, *Simulation eines Wafer-Biegetests durch Verwendung der von Kármán'schen Plattentheorie für kubisch anisotrope Materialien*, Oberseminar Numerik/Analysis, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, January 9.
55. ———, *Diffusion induced inelastic deformation of crystalline solid mixtures*, Sixth GAMM Seminar on Microstructures, January 12–13, WIAS, Berlin, January 13.
56. ———, *Diffusion in single crystal gallium arsenide in the surrounding area of a moving solid-gaseous interface*, 8th Hirschegg Workshop on Conservation Laws, September 9–15, September 13.
57. ———, *Modellierung der Präzipitat-Entwicklung durch Arsen-Diffusion in GaAs*, Oberseminar, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, December 13.
58. M. Elagin, *Comparison of some methods for the adaptive estimation of univariate time series parameters*, Cemapre Conference on Advances in Semiparametric Methods and Applications, Satellite meeting of ISI 2007, August 20–21, Lisbon, Portugal, August 21.
59. J. Elschner, *Variational approach to rough surface scattering*, University of Tokyo, Department of Mathematical Sciences, Japan, February 5.
60. ———, *On uniqueness in inverse scattering with finitely many incident waves*, Workshop "Inverse Problems in Wave Scattering", March 5–9, Mathematisches Forschungsinstitut Oberwolfach, March 6.
61. ———, *On uniqueness in inverse scattering by obstacles and diffraction gratings*, Conference "Boundary Elements — Theory and Applications" (Beta 2007), May 22–24, Leibniz Universität Hannover, May 22.
62. P. Ferrari, *Les processus universels d'Airy et le processus d'exclusion asymétrique*, University of Geneva, Faculty of Science, Switzerland, January 12.

63. ———, *A stochastic growth of an interface on a plane: Fluctuations for the KPZ universality class*, BRG Workshop on Stochastic Models from Biology and Physics, March 30–31, Universität Bielefeld, Fakultät für Mathematik, March 30.
64. ———, *A stochastic growth of an interface on a plane: Fluctuations for the KPZ universality class*, Technische Universität München, Zentrum Mathematik, April 4.
65. ———, *A stochastic growth of an interface on a plane: Fluctuations for the KPZ universality class*, Meeting on Large Quantum Systems, June 11–15, Warwick University, Department of Mathematics, Coventry, UK, June 13.
66. ———, *Transition between Airy$_1$ and Airy$_2$ processes and TASEP fluctuations*, Conference on Interactions of Random Matrix Theory, Integrable Systems and Stochastic Processes, June 24–28, University of Utah, Department of Mathematics, Snowbird, USA, June 27.
67. ———, *A stochastic growth of an interface on a plane: Fluctuations for the KPZ universality class*, Research Program of the IAS/Park City Mathematics Institute (PCMI) 2007 Summer School, July 1–21, Institute for Advanced Study, Park City Mathematics Institute, Park City, USA, July 6.
68. ———, *Around the universality of the Airy$_1$ process*, Workshop “Large Scale Stochastic Dynamics”, August 26 – September 1, Mathematisches Forschungsinstitut Oberwolfach, August 29.
69. ———, *Two Airy processes and their transition in the asymmetric exclusion process*, Conference on “Random and Integrable Models in Mathematics and Physics”, September 11–15, Solvay Institute, Brussels, Belgium, September 15.
70. ———, *Universality of the Airy processes along space-like paths*, CEA-Saclay, Paris, November 29.
71. ———, *Universality of the Airy processes along space-like paths*, Universität Leipzig, Fakultät für Mathematik und Informatik, December 10.
72. J. Fuhrmann, *Finite volume schemes for nonlinear convection-diffusion problems based on the solution of local Dirichlet problems*, Freie Universität Berlin, January 19.
73. ———, *Voronoï box based finite volume methods for systems of reaction-diffusion-convection equations*, Université de Provence, Laboratoire d’Analyse, Topologie, Probabilités, Marseille, France, April 10.
74. ———, *Aspects of finite volume methods in numerical modelling of electrochemical devices*, Université de Marne-la-Vallée, Département de Mathématiques, Champs-sur-Marne, France, April 13.
75. ———, *Voronoï box based finite volume methods in scientific computing*, Institut Français du Pétrole, Rueil-Malmaison, France, April 24.
76. ———, *Finite volume methods in numerical modelling of electrochemical devices*, Université Paris-Sud 11, Orsay, France, April 25.
77. ———, *Numerical modelling of electrochemical flow cells*, Université Blaise Pascal, Clermont-Ferrand, France, May 4.
78. ———, *Issues in numerical modelling of differential electrochemical mass spectroscopy in flow cells*, Sixth Negev Applied Mathematical Workshop, July 1–5, Ben Gurion University of the Negev, Jacob Blaustein Institute for Desert Research, Sede Boqer Campus, Israel, July 3.
79. P. Gapeev, *Constructing jump analogues of diffusions and applications to finance*, Seminar “Financial Mathematics and Applied Probability”, King’s College London, Financial Mathematics, UK, January 23.
80. ———, *Convertible bonds in structural and reduced form models*, Seminar “Finance and Stochastic”, Imperial College London, Department of Mathematics, UK, January 24.
81. ———, *Perpetual options in jump-diffusion models: Barrier, lookback and credit options*, Seminar “Risk and Stochastics”, London School of Economics, Department of Statistics, UK, January 25.
82. ———, *Bayesian sequential testing and disorder problems for some diffusion processes*, Seminar “Statistical Laboratory”, University of Cambridge, Centre for Mathematical Sciences, UK, January 26.
83. ———, *Pricing perpetual options in jump-diffusion models*, Mathematisches Kolloquium, Universität Dortmund, February 22.
84. ———, *Valuation of American options in jump-diffusion models*, Seminar for Mathematical Economics, Universität Bielefeld, May 22.

85. ———, *Constructing jump analogues of diffusions and application to finance*, Technische Universität Wien, Financial and Actuarial Mathematics, Austria, June 12.
86. K. Gärtner, *Applications at WIAS — Overview and one example in some detail: The van Roosbroeck system and discretizations preserving qualitative properties*, Technische Universität München, Walter-Schottky-Institut, February 6.
87. ———, *Dissipative discretization schemes for phase-separation models*, Ben Gurion University of the Negev, Jacob Blaustein Institute for Desert Research, Sede Boqer Campus, Israel, March 6.
88. ———, *The van Roosbroeck system, bounded discrete steady state solutions on boundary conforming Delaunay grids*, Sixth Negev Applied Mathematical Workshop, July 1–5, Ben Gurion University of the Negev, Jacob Blaustein Institute for Desert Research, Sede Boqer Campus, Israel, July 4.
89. ———, *Existence of bounded discrete steady state solutions of the van Roosbroeck system on boundary conforming Delaunay grids*, 7th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD'07), September 24–27, University of Delaware, Newark, USA, September 26.
90. E. Giacomini, *Statistics and risk aversion*, Cemapre Conference on Advances in Semiparametric Methods and Applications, Satellite meeting of ISI 2007, August 20–21, Lisbon, Portugal, August 20.
91. ———, *Inhomogeneous dependence modelling with time varying copulae*, Forum Seminar, Charles University of Prague, Department of Probability and Mathematical Statistics, Czech Republic, November 14.
92. ———, *Introduction to the statistical software XploRe*, Seminar "Computational Environment for Statistics", Charles University of Prague, Department of Probability and Mathematical Statistics, Czech Republic, November 21.
93. J.A. Griepentrog, *On the analysis of nonlocal phase separation processes in multicomponent systems*, International Conference on Differential Equations (EQUADIFF 07), Minisymposium on Nonlinear Diffusion Equations, August 5–11, Vienna University of Technology, Austria, August 6.
94. C. Guhlke, *Non-linear elastic membrane shells for incompressible Mooney–Rivlin materials and non-linear phenomena of rubber*, Workshop "Multiscale Problems in Three Applications", May 29 – June 1, WIAS, May 31.
95. R. Henrion, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen: Anwendungen, Modelle, Struktur und Numerik*, Technische Universität Ilmenau, Institut für Automatisierung und Systemtechnik, January 11.
96. ———, *Chance-constrained stochastic programming*, Spring School on Stochastic Programming: Theory and Applications, University of Bergamo, Italy, April 12.
97. ———, *Distance to uncontrollability for convex processes*, International Congress "Mathematical Methods in Economics and Industry" (MMEI 2007), June 3–7, Herlany, Slovakia, June 5.
98. ———, *Szenario-Reduktion bezüglich Diskrepanz-Metriken*, Universität Duisburg-Essen, Fachbereich Mathematik, June 20.
99. ———, *Avoidance of random obstacles by means of probabilistic constraints*, 6th International Congress on Industrial and Applied Mathematics (ICIAM 2007), July 16–20, ETH Zürich, Switzerland, July 16.
100. ———, *Contraintes en probabilité: synthèse bibliographique et approche à la situation dynamique*, Electricité de France R&D, Clamart, France, November 28.
101. E. Holzbecher, *Groundwater flow and transport modelling using COMSOL/FEMLAB, Part II (block lecture)*, 15 talks, Polish Geological Institute, Pomeranian Branch, Szczecin, February 19–23.
102. ———, *Groundwater flow and transport modelling using COMSOL/FEMLAB, Part III (block lecture)*, 15 talks, Polish Geological Institute, Pomeranian Branch, Szczecin, July 2–6.
103. ———, *Double diffusive convection above a saltdome*, 2nd MELA (Morphotectonic map of the European Lowland Area) Conference "Glaciotectonic structures, palaeobasins and neotectonic setting", August 27–31, Lithuanian Geological Survey, Vilnius, August 30.
104. ———, *Modelling of direct methanol fuel cells for microelectronical devices*, World Hydrogen Technologies Convention, November 4–7, Montecatini Terme, Italy, November 7.
105. ———, *Groundwater flow and transport modelling using COMSOL/FEMLAB, Part IV (block lecture)*, 15 talks, Polish Geological Institute, Pomeranian Branch, Szczecin, December 17–21.

106. D. Hömberg, *On a thermomechanical phase transition model for the heat treatment of steel*, Universidad de Cádiz, Departamento de Matemáticas, Puerto Real, Spain, January 15.
107. ———, *Mathematical tools for the simulation and control of heat treatments*, Delphi, Puerto Real, Spain, January 16.
108. ———, *Optimal control of semilinear parabolic equations and an application to laser material treatments (part I)*, University of Tokyo, Department of Mathematical Sciences, Japan, February 21.
109. ———, *Optimal control of semilinear parabolic equations and an application to laser material treatments (part II)*, University of Tokyo, Department of Mathematical Sciences, Japan, February 22.
110. ———, *Mathematics for steel production and manufacturing*, Nippon Steel, Kimitsu, Japan, March 1.
111. ———, *On a thermomechanical phase transition model for the heat treatment of steel*, Fudan University, Department of Mathematics, Shanghai, China, March 5.
112. ———, *A short course on PDE-constrained optimal control*, 8 talks, Universitá degli Studi di Milano, Dipartimento di Matematica, Italy, March 20–30.
113. ———, *Mathematics for complex production processes*, Comau, Turin, Italy, March 23.
114. ———, *Solid-solid phase transitions in steel — modeling, simulation and optimal control*, Universitá di Pavia, Dipartimento di Matematica, Italy, March 27.
115. ———, *Thermomechanical phase transition models — analysis, optimal control and industrial applications*, University of Oxford, Oxford Centre for Industrial and Applied Mathematics, UK, October 11.
116. ———, *Phase transition models for multiphase steels*, Industrial and Interdisciplinary Workshop "Problems Related to the Manufacture of Multiphase Steels", University of Oxford, Oxford Centre for Industrial and Applied Mathematics, UK, November 2.
117. D. Hömberg, D. Kern, *Optimal control of a thermomechanical model of phase transitions in steel*, 6th International Congress on Industrial and Applied Mathematics (ICIAM 2007), July 16–20, ETH Zürich, Switzerland, July 19.
118. E. Höschele, *Simulation der Spaltströmung: nicht-Newtonsche Flüssigkeit, feste Rollen*, Océ, München, July 23.
119. ———, *Einbau des Elastizitätsmodells in NAVIER*, Océ, München, September 19.
120. H.-Chr. Kaiser, *A drift-diffusion model of transient Kohn–Sham theory*, First Joint International Meeting between the American Mathematical Society and the Polish Mathematical Society, Special Session "Mathematics of Large Quantum Systems", July 31 – August 3, University of Warsaw, Poland, August 3.
121. J. Kampen, *Closed form analytic expansion formulas for characteristic functions of affine jump diffusion processes*, Workshop on Numerics in Finance, November 5–6, Commerzbank AG, Frankfurt/Main, November 6.
122. D. Kern, *Optimal control of a thermo-mechanical model of phase transitions in steel*, 13th Czech-French-German Conference on Optimization, September 17–21, Heidelberg, September 20.
123. D. Knees, *Energy release rate for cracks in finite-strain elasticity*, Workshop "Analysis and Numerics of Rate-Independent Processes", February 26 – March 2, Mathematisches Forschungsinstitut Oberwolfach, February 27.
124. ———, *Energy release rate for cracks in finite-strain elasticity*, Arbeitsgemeinschaft Mikrostrukturen, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, April 17.
125. ———, *Global spatial regularity for weak solutions of an elasto-viscoplastic model*, Seminar "Numerische Mathematik", Technische Universität Graz, Institut für Numerische Mathematik, Austria, May 14.
126. A. Kolodko, *Iterative procedure for pricing Bermudan options*, University of Technology, Sydney, Department of Mathematical Sciences, Australia, March 22.
127. M. Korzec, *QR decomposition based linear algebra and QP aspects of the total quasi-Newton idea*, Gemeinsame Jahrestagung der Deutschen Mathematiker-Vereinigung und der Gesellschaft für Didaktik der Mathematik 2007, March 25–30, Humboldt-Universität zu Berlin, March 30.
128. Ch. Kraus, *On jump conditions at phase interfaces*, Oberseminar über Angewandte Mathematik, December 10–15, Universität Freiburg, Abteilung für Angewandte Mathematik, December 11.

129. P. Krejčí, *Energy estimates for the Preisach model*, 6th International Symposium on Hysteresis Modeling and Micromagnetics (HMM-07), June 4–6, Naples, Italy, June 5.
130. ———, *Dimensional reduction in oscillating thin elastoplastic bodies*, Direct, Inverse and Control Problems for PDE's (DICOP '07), June 25–28, Università di Bologna, Dipartimento di Matematica, Rome, Italy, June 25.
131. ———, *Maximal entropy production principle in nonsmooth evolution systems (in Czech)*, Seminar "Mathematics in Colleges", September 3–5, Herbertov, Czech Republic, September 4.
132. ———, *Forgetting and memory (in Czech)*, 3rd Annual Meeting of the Mathematical Institute of the Czech Academy of Sciences, September 24–27, Hejnice, Czech Republic, October 25.
133. ———, *Well-posedness and long time behavior of spatially nonlocal phase-field systems*, International Conference on Free Boundary Problems (FBP2007) "Nonlinear Phenomena with Energy Dissipation: Mathematical Analysis, Modelling and Simulation", November 26–30, Chiba University, Japan, November 29.
134. ———, *Quasilinear hyperbolic equations with hysteresis*, Seminar on Mathematics for various disciplines, University of Tokyo, Graduate School of Mathematical Sciences, Japan, December 4.
135. Ch. Lechner, *Simulationen zum Einsatz eines Wandermagnetfeldes in der $A_{III}B_V$-Czochralski-Züchtung*, 5. Workshop "Angewandte Simulation in der Kristallzüchtung", April 25–26, Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung e.V. (DGKK), Iphofen, April 25.
136. ———, *Numerische Simulation von Czochralski-Züchtung unter dem Einfluss eines Wandermagnetfeldes*, KRIST$\widehat{MAG}$-Statusseminar, June 18–20, Berlin, June 19.
137. A. Linke, *Lowest-order Scott–Vogelius elements for the incompressible Navier–Stokes equation*, Universität Göttingen, Institut für Numerische und Angewandte Mathematik, January 10.
138. P. Mathé, *Discretization of inverse problems*, Workshop on Applied Analysis and Differential Equations, July 5–6, Vietnamese Academy of Science and Technology, Hanoi, July 5.
139. ———, *Local analysis of inverse problems*, Chemnitz Symposium on Inverse Problems 2007, September 27–28, Technische Universität Chemnitz, September 27.
140. Ch. Meyer, *Finite-element error analysis of state-constrained optimal control problems*, Second Chilean Workshop on Numerical Analysis of Partial Differential Equations (WONAPDE 2007), January 16–19, Concepcion, Chile, January 16.
141. ———, *Optimal control of nonlocal radiation*, Escuela Politécnica Nacional, Departamento de Matemática, Quito, Ecuador, January 24.
142. ———, *Finite-element approximation of state-constrained optimal control problems*, Workshop "Optimierungsmethoden, Approximation und Adaptivität bei Optimierungsproblemen mit partiellen Differentialgleichungen", March 7–9, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, March 8.
143. ———, *Well-posedness of a state constrained optimal control problem*, Gemeinsame Jahrestagung der Deutschen Mathematiker-Vereinigung und der Gesellschaft für Didaktik der Mathematik 2007, March 26–30, Humboldt-Universität zu Berlin, March 27.
144. ———, *Optimal control of the thermistor problem*, Universität Bremen, Fachbereich 3 – Informatik, May 30.
145. ———, *Optimal control of heat transfer with radiation interface conditions and pointwise state constraints*, SIAM Conference on Control and Its Applications, June 29 – July 1, San Francisco, USA, June 30.
146. ———, *Optimal control of the thermistor problem*, 23rd IFIP TC7 Conference on System Modelling and Optimization, July 23–27, Crakow, Poland, July 26.
147. ———, *Optimal control of the thermistor problem*, 13th Czech-French-German Conference on Optimization, September 18–21, Heidelberg, September 20.
148. A. Mielke, *Classical rate-independent models including elastoplasticity*, Lipschitz Lectures "Modeling and analysis of rate-independent processes", January 8–23, Rheinische Friedrich-Wilhelms-Universität, Institut für Angewandte Mathematik, Bonn, January 8.
149. ———, *The energetic formulation via functionals*, Lipschitz Lectures "Modeling and analysis of rate-independent processes", January 8–23, Rheinische Friedrich-Wilhelms-Universität, Institut für Angewandte Mathematik, Bonn, January 9.

150. ———, *Viscous and kinetic regularizations*, Lipschitz Lectures "Modeling and analysis of rate-independent processes", January 8–23, Rheinische Friedrich-Wilhelms-Universität, Institut für Angewandte Mathematik, Bonn, January 15.
151. ———, *Applications in material models*, Lipschitz Lectures "Modeling and analysis of rate-independent processes", January 8–23, Rheinische Friedrich-Wilhelms-Universität, Institut für Angewandte Mathematik, Bonn, January 16.
152. ———, *Relaxation and Gamma convergence for rate-independent processes*, Lipschitz Lectures "Modeling and analysis of rate-independent processes", January 8–23, Rheinische Friedrich-Wilhelms-Universität, Institut für Angewandte Mathematik, Bonn, January 22.
153. ———, *Evolution of microstructures and numerical approaches*, Lipschitz Lectures "Modeling and analysis of rate-independent processes", January 8–23, Rheinische Friedrich-Wilhelms-Universität, Institut für Angewandte Mathematik, Bonn, January 23.
154. ———, *Weak-convergence methods for Hamiltonian multiscale problems*, Sixth Workshop on Multiscale Problems in Quantum Mechanics, February 8–9, Universität Tübingen, February 9.
155. ———, *On the energetic formulation of rate-independent processes and applications*, 6th Meeting of MULTIMAT, a Marie Curie Research Training Network, April 19–21, Institute of Physics/Mathematical Institute, Academy of Sciences of the Czech Republic, Prague, April 19.
156. ———, *Gamma convergence for rate-independent processes with application to damage*, Workshop "Phase Transitions", June 4–8, Mathematisches Forschungsinstitut Oberwolfach, June 5.
157. ———, *Global existence for a model with complete damage*, Joint International Meeting UMI-DMV 2007, minisymposium "Variational problems in continuum mechanics", June 18–22, Università degli Studi di Perugia, Dipartimento di Matematica e Informatica, Italy, June 20.
158. ———, *Local versus global stability in rate-independent processes*, Joint International Meeting UMI-DMV 2007, minisymposium "Phase transitions and hysteresis in free boundary problems", June 18–22, Università degli Studi di Perugia, Dipartimento di Matematica e Informatica, Italy, June 21.
159. ———, *Existence of energetic solutions in finite-strain plasticity*, 6th International Congress on Industrial and Applied Mathematics (ICIAM), minisymposium "Mathematical Aspects of Materials Science", July 16–20, ETH Zürich, Switzerland, July 18.
160. ———, *Rate-independent processes and a model with complete damage*, International Conference on Differential Equations (EQUADIFF 07), Minisymposium on Rate-Independent Evolutions and Material Modeling, August 5–11, Vienna University of Technology, Austria, August 9.
161. ———, *Modelling of rate-independent hysteresis effects in materials*, 4 talks, Workshop "Structures of the mechanics of complex bodies", October 1–7, Centro di Ricerca Matematica "Ennio De Giorgi", Pisa, Italy, October 1–6.
162. ———, Γ*-convergence for evolutionary problems*, 4 talks, Autumn School "Analysis of Multiphase Problems" of the Research Training Group "Analysis, Numerics, and Optimization of Multiphase Problems" (GRK 1128), Nečas Center for Mathematical Modeling and Institute of Information Theory and Automation, Prague, Czech Republic, October 8–12.
163. ———, *Plasticity as a limit for a chain with viscous, stochastic, bistable springs*, Workshop on Microscopic Origins of Dissipation and Noise, October 31 – November 3, University of Bath / Leipzig University, Leipzig, November 1.
164. ———, *Global existence for rate-independent gradient plasticity at finite strain*, Workshop on Rate-Independence, Homogenization and Multiscaling, November 15–17, Centro di Ricerca Matematica "Ennio De Giorgi", Pisa, Italy, November 17.
165. ———, *Wiggly energy landscapes and the origin of rate-independent friction*, Istituto di Matematica Applicata e Tecnologie Informatiche – Consiglio Nazionale delle Ricerche, Pavia, Italy, November 20.
166. M. Naldzhieva, *On a continuous approximation of a thermodynamically consistent Becker–Döring model*, Universität Magdeburg, Institut für Analysis und Numerik, December 3.
167. H. Neidhardt, *On a quantum transmitting Schrödinger–Poisson system*, Mini-Workshop on PDE's and Quantum Transport, March 12–16, Aalborg University, Department of Mathematical Sciences, Denmark, March 15.

168. ———, *Boundary triplets and scattering*, International Conference "Modern Analysis and Applications" (MAA 2007), April 9–14, Institute of Mathematics, Economics and Mechanics of Odessa National I.I. Mechnikov University, Ukraine, April 13.
169. ———, *On a quantum transmitting Schrödinger–Poisson system*, Mathematisches Kolloquium, Technische Universität Clausthal, Institut für Mathematik, Clausthal, April 25.
170. ———, *On Eisenbud's and Wigner's R-matrix: A general approach*, 10th Quantum Mathematics International Conference (QMath 10), September 10–15, Institute of Mathematics "Simion Stoilow" of the Romanian Academy, Moeciu, Romania, September 11.
171. ———, *On trace formula and Birman–Krein formula for pairs of extensions*, 7th Workshop on Operator Theory in Krein Spaces and Spectral Analysis, December 13–16, Technische Universität Berlin, Institut für Mathematik, December 13.
172. R. Nürnberg, *2D-Simulation eines neuen Solarzellkonzeptes für die Anwendung in der Photovoltaik*, Halbleiter-Kolloquium, Hahn-Meitner-Institut, Abteilung SE2 (Heterogene Materialsysteme), Berlin, May 24.
173. L. Panizzi, *Modelling, analysis, and simulation of case hardening*, 6th International Congress on Industrial and Applied Mathematics (ICIAM 2007), July 16–20, ETH Zürich, Switzerland, July 19.
174. A. Petrov, *Thermally driven phase transformation in shape-memory alloys*, Workshop "Analysis and Numerics of Rate-Independent Processes", February 26 – March 2, Mathematisches Forschungsinstitut Oberwolfach, February 27.
175. M. Pietrzyk, *How to describe ultrashort pulses when the NSE does not apply?*, Optics Lab, University of Vigo, Spain, July 2.
176. ———, *Multisymplectic analysis of the short pulse equation*, 10th International Conference on Differential Geometry and Its Application, August 27–31, Olomouc, Czech Republic, August 28.
177. J. Polzehl, *Structural adaptive smoothing methods*, Gemeinsames Kolloquium des Fachbereichs Statistik und des SFB 475, Universität Dortmund, January 30.
178. ———, *Structural adaptive smoothing methods and related topics*, Kick-off Meeting eVITA project, Tromsø, Norway, February 15.
179. ———, *Propagation-separation procedures for image processing*, International Workshop on Image Analysis in the Life Sciences, Theory and Applications, February 28 – March 2, Johannes Kepler Universität Linz, Austria, March 2.
180. ———, *Structural adaptive smoothing in imaging problems*, Spring Seminar Series, University of Minnesota, School of Statistics, College of Liberal Arts, USA, May 24.
181. ———, *Structural adaptive smoothing: Images, fMRI and DWI*, Workshop on Algorithms in Complex Systems, September 24–26, EURANDOM, Eindhoven, The Netherlands, September 24.
182. ———, *Structural adaptive smoothing procedures by propagation-separation methods*, Final meeting of the DFG Priority Program 1114, November 7–9, Freiburg, November 7.
183. P.N. Racec, E.R. Racec, U. Wulf, *Linear response theory for open two-terminal quantum systems*, 10th Quantum Mathematics International Conference (QMath 10), September 10–15, Institute of Mathematics "Simion Stoilow" of the Romanian Academy, Moeciu, Romania, September 13.
184. M. Radziunas, *Travelling wave modelling of the semiconductor ring lasers*, European Semiconductor Lasers Workshop (ESLW 2007), September 14–15, Fraunhofer Heinrich-Hertz-Institut, Berlin, September 14.
185. A. Rathsfeld, *Sensitivity analysis for indirect measurement in scatterometry and the reconstruction of periodic grating structures*, 6th International Congress on Industrial and Applied Mathematics (ICIAM 2007), July 16–20, ETH Zürich, Switzerland, July 20.
186. J. Rehberg, *Operator functions inherit monotonicity*, Mini-Workshop on PDE's and Quantum Transport, March 12–16, Aalborg University, Department of Mathematical Sciences, Denmark, March 14.
187. ———, *Über Schrödinger-Poisson-Systeme*, Chemnitzer Mathematisches Colloquium, Technische Universität Chemnitz, Fakultät für Mathematik, May 24.

188. ———, *On Schrödinger–Poisson systems*, International Conference "Nonlinear Partial Differential Equations" (NPDE 2007), September 10–15, Institute of Applied Mathematics and Mechanics of NASU, Yalta, Ukraine, September 13.
189. ———, *Maximal parabolic regularity on Sobolev spaces*, The Eighteenth Crimean Autumn Mathematical School-Symposium (KROMSH-2007), September 17–29, Laspi-Batiliman, Ukraine, September 18.
190. ———, *Maximale parabolische Regularität für Divergenz-Operatoren auf Sobolevräumen*, Oberseminar "Nichtlineare Analysis", Universität Köln,Mathematisches Institut, December 3.
191. A. Rohde, *Adaptive goodness-of-fit tests based on signed ranks*, Seminar "Econometrics and Statistics", Université Libre de Bruxelles, European Center for Advanced Research in Economics and Statistics, Belgium, December 13.
192. K.K. Sabelfeld, *Monte Carlo methods for stochastic PDEs*, VI IMACS Seminar on Monte Carlo Methods (MCM 2007), June 18–21, University of Reading, UK, June 20.
193. ———, *Random walk methods for solving stochastic elasticity problems*, VI IMACS Seminar on Monte Carlo Methods (MCM 2007), June 18–21, University of Reading, UK, June 20.
194. ———, *A stratified sampling simulation of coagulation processes and application to crystal growth*, Workshop "Coagulation and Fragmentation Models", September 23–29, Mathematisches Forschungsinstitut Oberwolfach, September 25.
195. A. Schliwa, *Electronic properties of self-organized quantum dots*, Seminar "Halbleiterquantenpunkte", Leibniz-Institut für Festkörper- und Werkstoffforschung (IWF), Institut für Integrative Nanowissenschaften, Dresden, April 17.
196. ———, *Optical QD properties as quantitative fingerprints of structural and chemical properties*, 2nd SANDiE Workshop "Characterization and modelling of self-assembled semiconductor nanostructures", December 12–14, CNRS-LPN (Laboratoire de Photonique et de Nanostructures) and Institut d'Electronique Fondamentale, Paris, France, December 12.
197. G. Schmidt, *Regularity of solutions to anisotropic elliptic transmission problems*, Fifth Singular Days, April 23–27, Luminy, France, April 24.
198. ———, *Integral equations for conical diffraction*, University of Liverpool, Department of Mathematics, UK, December 7.
199. J.G.M. Schoenmakers, *Policy iteration for American/Bermudan style derivatives*, 6th Winter school on Mathematical Finance, January 22–24, CongresHotel De Werelt, Lunteren, The Netherlands, January 23.
200. ———, *Iterative procedures for the Bermudan stopping problem*, International Multidisciplinary Workshop on Stochastic Modeling, June 25–29, Sevilla, Spain, June 26.
201. ———, *Enhanced policy iteration via scenario selection*, International Multidisciplinary Workshop on Stochastic Modeling, June 25–29, Sevilla, Spain, June 27.
202. ———, *True upper bounds for Bermudan style derivatives*, International Multidisciplinary Workshop on Stochastic Modeling, June 25–29, Sevilla, Spain, June 28.
203. ———, *Robust Libor modelling and calibration*, International Multidisciplinary Workshop on Stochastic Modeling, June 25–29, Sevilla, Spain, June 29.
204. ———, *Policy iterated lower bounds and linear MC upper bounds for Bermudan style derivatives*, Workshop on Quantitative Finance, November 15–16, HSH Nordbank-CAU, Kiel, November 15.
205. A. Segatti, *Attractors for evolution problems without uniqueness (in Italian)*, XVIII Congresso dell'Unione Matematica Italiana, September 24–29, Bari, Italy, September 28.
206. V. Spokoiny, *Modern nonparametric statistics*, 2 talks, Hejnice Seminar 2007 (Collaborative Research Center SFB 649 "Economic Risk"), February 8–10, International Centre for Spiritual Rehabilitation, Hejnice, Czech Republic, February 9.
207. ———, *Robust risk management. Accounting for nonstationarity and heavy tails*, Econometrics and Statistics Seminar, Tilburg University, The Netherlands, February 14.
208. ———, *Robust risk management. Accounting for nonstationarity and heavy tails*, Seminar "Statistique", Université de Rennes I, Institut de Recherche Mathématique, France, March 9.

209. ———, *Foundations and applications of modern nonparametric statistics*, 3 talks, Ruhr Graduate School in Economics, Essen, April 2.
210. ———, *Robust risk management. Accounting for nonstationarity and heavy tails*, RMI Research Workshop Series, September 2–28, National University of Singapore, Risk Management Institute, September 7.
211. ———, *Adaptive estimation in a linear inverse problem*, Workshop "Reassessing the Paradigms of Statistical Model-Building", October 21–25, Mathematisches Forschungsinsitut Oberwolfach, October 23.
212. J. Sprekels, *Elastic-ideally plastic beams and 1D Prandtl–Ishlinskii hysteresis operators*, Workshop "Phase Transitions", June 3–9, Mathematisches Forschungsinstitut Oberwolfach, June 7.
213. ———, *Models of phase transitions and hysteresis operators*, Joint International Meeting UMI-DMV 2007, minisymposium "Phase transitions and hysteresis in free boundary problems", June 18–22, Università degli Studi di Perugia, Dipartimento di Matematica e Informatica, Italy, June 21.
214. ———, *How computers and modern mathematics change our world*, Fourth Annual Meeting of the STS (Science and Technology in Society) Forum, October 7–9, Kyoto, Japan, October 8.
215. H. Stephan, *Linear evolution systems conserving positivity*, Research Seminar of the Mathematical Division, B. Verkin Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine, July 4.
216. ———, *Time behavior of positive semigroups in various Banach spaces*, The Eighteenth Crimean Autumn Mathematical School-Symposium (KROMSH-2007), September 17–29, Laspi-Batiliman, Ukraine, September 21.
217. K. Tabelow, *Structural adaptive smoothing in medical imaging*, Seminar "Visualisierung und Datenanalyse", Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB), January 30.
218. ———, *Structural adaptive signal detection in fMRI and structure enhancement in DTI*, International Workshop on Image Analysis in the Life Sciences, Theory and Applications, February 28 – March 2, Johannes Kepler Universität Linz, Austria, March 2.
219. ———, *Improving data quality in fMRI and DTI by structural adaptive smoothing*, Cornell University, Weill Medical College, New York, USA, June 18.
220. A. Vladimirov, *Autosolitons in optical devices with transverse refractive index modulation*, International Conference on Coherent and Nonlinear Optics/International Conference on Lasers, Applications, and Technologies (ICONO/LAT 2007), May 28 – June 1, Minsk, Belarus, May 29.
221. ———, *Passive mode-locking in quantum dot lasers*, Joint Seminar on Quantum Optics, St. Petersburg State University and Herzen State Pedagogical University, Russia, December 26.
222. B. Wagner, *Sharp-interface models for dewetting films*, Workshop "Multiscale Problems in Three Applications", May 29 – June 1, WIAS, May 31.
223. ———, *Sharp-interface models and contact line instabilities for dewetting films*, Summer Workshop 2007 of the DFG Priority Program SPP 1164 "Nano- and Microfluidics", August 1–3, Bad Honnef, August 2.
224. ———, *Contact-line instability for dewetting liquid films and sharp-interface models*, EUROMECH 490: Workshop "Dynamics and Stability of Thin Liquid Films and Slender Jets, The Institute for Mathematical Sciences, Imperial College London, UK, September 19.
225. W. Weiss, *Simulationsbasierte Regelung der Laserhärtung von Stahl*, Ruhr-Universität Bochum, Institut für Werkstoffe, May 30.
226. ———, *Control of laser surface hardening*, 6th International Congress on Industrial and Applied Mathematics (ICIAM 2007), July 16–20, ETH Zürich, Switzerland, July 19.
227. M. Wolfrum, *Delay differential equations with large delay*, Dynamical Systems Seminar, University of Minnesota, School of Mathematics, Minneapolis, USA, March 5.
228. X. Yao, *Metastability of the Kawasaki dynamics on the random graphs*, Meeting of the Dutch-German Research Group on Mathematics of Random Spatial Models from Physics and Biology, November 2–3, EURANDOM, Eindhoven, The Netherlands, November 3.

A.8.2 Talks for a More General Public

1. I. Bremer, *Wir zeigen dem Industrieroboter, wo's lang geht*, 12. Berliner Tag der Mathematik (12th Berlin Day of Mathematics), Technische Fachhochschule Berlin, May 5.

2. P. Ferrari, *Universalität: Ein unerwarteter Zusammenhang zwischen Kristallflächen und Verkehrsstaus*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2007, WIAS, June 9.
3. D. Hömberg, *Mathematik — Rohstoff für die Industriegesellschaft*, 15 Jahre Forschungsverbund Berlin, Urania, Berlin, March 12.
4. Ch. Meyer, *Auf der Suche nach dem Optimum — Was kommt nach der Kurvendiskussion?*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2007, WIAS, Berlin, June 9.
5. A. Mielke, *Warum sind moderne Materialien schlau?*, MathInside — Mathematik (nicht nur) für Schüler, Urania, Berlin, March 20.
6. G. Reinhardt, *Berufsausbildung "Mathematisch-technische/r Softwareentwickler/in" am Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)*, Berufskundliche Vortragsreihe am Berufsinformationszentrum, Berlin, September 13.
7. A. Steinbrecher, *Warum studierst Du denn Mathematik? — Es gibt doch Computer*, 12. Berliner Tag der Mathematik (12th Berlin Day of Mathematics), Technische Fachhochschule Berlin, May 5.
8. K. Tabelow, *Den Gedanken auf der Spur – Bildgebende Verfahren in der Hirnforschung*, 12. Berliner Tag der Mathematik (12th Berlin Day of Mathematics), Technische Fachhochschule Berlin, May 5.
9. W. Weiss, *Thermodynamische Betrachtungen zur Hölle und zum Himmel*, Mathematik-Schau des DFG-Forschungszentrums Matheon, Technische Universität Berlin, November 30.

A.8.3 Posters

1. K. Afanasiev, A. Münch, B. Wagner, *The role of slippage in thin liquid films and droplets on rigid and viscoelastic substrates*, Review Days of the DFG Priority Program SPP 1164: "Nano- & Microfluidics: Bridging the Gap between Molecular Motion and Continuum Flow", Bonn, December 5–7.
2. U. Bandelow, A. Demircan, M. Kroh, B. Hüttl, *Appearance of solitonic effects during pulse compression in the normal dispersion regime*, Rio de la Plata Workshop on Noise, Chaos and Complexity in Lasers and Nonlinear Optics, Punta del Este, Uruguay, December 3–6.
3. A. Demircan, U. Bandelow, *Interplay between soliton fission and modulation instability*, European Conference on Lasers and Electro-Optics 2007/International Quantum Electronics Conference (CLEOE-IQEC 2007), München, June 17–22.
4. A. Demircan, U. Bandelow, B. Hüttl, M. Kroh, *Generation of new frequencies by pulse splitting*, 33rd European Conference and Exhibition on Optical Communication (ECOC 2007), Berlin, September 16–20.
5. J. Fuhrmann, K. Gärtner, E. Holzbecher, H. Langmach, A. Linke, H. Zhao, *Numerical models of electrochemical devices*, Conference "From Physical Understanding to Novel Architectures of Fuel Cells", Trieste, Italy, May 21–25.
6. E. Holzbecher, S. Krumbholz, *Modelling of channel — Gas diffusion layer systems*, COMSOL Conference 2007, Grenoble, France, October 23–24.
7. A. Bradji, E. Holzbecher, *On the convergence order of COMSOL solutions*, COMSOL Conference 2007, Grenoble, France, October 23–24.
8. E. Holzbecher, K. Gärtner, J. Fuhrmann, H. Langmach, *Numerical solution of Stefan–Maxwell systems*, Young Scientists Workshop Transport Phenomena in Fuel Cells, University of Victoria, Canada, May 4–5.
9. 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)*, The 15th International Conference on Crystal Growth, Salt Lake City, USA, August 12–17.
10. O. Klein, P. Philip, J. Geiser, D. Siche, J. Wollweber, *Numerical investigation of the influence of an anisotropic insulation felt on the temperature field in a PVT growth apparatus*, The 15th International Conference on Crystal Growth, Salt Lake City, USA, August 12–17.
11. H.-J. Mucha, *Model-based pairwise cluster analysis of weighted observations*, Gemeinsame Jahrestagung der Deutschen Mathematiker-Vereinigung und der Gesellschaft für Didaktik für Mathematik 2007, Humboldt-Universität zu Berlin, March 25–30.

12. H.-G. BARTEL, J. DOLATA, H.-J. MUCHA, *Visualizations of archaeometric data on the basis of statistcal analysis of Roman bricks and tiles*, 35th Annual Conference on Computer Applications and Quantitative Methods in Archaeology, Berlin, April 2–6.
13. M. PIETRZYK, *Properties of ultrashort pulses in silica fibers*, ATTO 07 — International Workshop and 391th WWE-Heraeus Seminar Attosecond Physics, Dresden, July 31 – August 4.
14. M. RADZIUNAS, *Simulation and analysis of the multimode model for semiconductor ring lasers*, PHASE Conference, Metz, France, March 28–30.
15. M. RADZIUNAS, U. TROPPENZ, J. KREISSL, *Tailoring single-mode DFB laser with integrated passive feedback section for direct modulation applications*, European Conference on Lasers and Electro-Optics, 2007/International Quantum Electronics Conference (CLEOE-IQEC 2007), Munich, June 17–22.
16. K. TABELOW, J. POLZEHL, H.U. VOSS, *Increasing SNR in high resolution fMRI by spatially adaptive smoothing*, Human Brain Mapping Conference 2007, Chicago, USA, June 10–14.
17. ———, *Reducing the number of necessary diffusion gradients by adaptive smoothing*, Human Brain Mapping Conference 2007, Chicago, USA, June 10–14.
18. A. MÜNCH, B. WAGNER, *Mathematical modeling, analysis, numerical simulation of thin films and droplets on rigid and viscoelastic substrates, emphasizing the role of slippage*, Summer Workshop 2007 of the Priority Program SPP 1164 “Nano- and Microfluidics”, Bad Honnef, August 1–3.
19. H. ZHAO, J. FUHRMANN, H. LANGMACH, E. HOLZBECHER, A. LINKE, *Flow, transport and reactions in a thin layer flow cell*, Young Scientists Workshop Transport Phenomena in Fuel Cells, University of Victoria, Canada, May 4–5.

A.9 Visits to other Institutions[4]

1. O. Zindy, Université Versailles Saint Quentin en Yvelines, France, November 21 – December 7.
2. A. Bianchi, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, March 13–27.
3. ———, Università di Roma Tre, Dipartimento di Matematica, Italy, April 10–19.
4. J. Borchardt, ALSTOM Power, Baden, Switzerland, August 20–24.
5. A. Bovier, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, December 19, 2006 – January 2, 2007.
6. ———, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, March 13–27.
7. ———, Princeton University, Department of Physics, USA, May 1–5.
8. ———, Peking University and Beijing Normal University, China, September 3–19.
9. ———, Chinese University of Mining and Technology, Xuzhou, China, September 20–25.
10. J. Elschner, University of Tokyo, Department of Mathematical Sciences, Japan, January 22 – February 9.
11. P. Ferrari, California Institute of Technology, CALTECH, Pasadena, USA, January 31 – February 14.
12. ———, Research Program of the IAS/Park City Mathematics Institute (PCMI) 2007 Summer School, Institute for Advanced Study, Park City Mathematics Institut, July 1–21.
13. J. Fuhrmann, Université de Marne-la-Vallée, Département de Mathématiques, Champs-sur-Marne, France, April 10 – May 4.
14. P. Gapeev, Imperial College London, Department of Mathematics, UK, January 16–30.
15. ———, Technische Universität Wien, Institut für Wirtschaftsmathematik, Austria, August 12–25.
16. K. Gärtner, Ben Gurion University of the Negev, Jacob Blaustein Institute for Desert Research, Sede Boqer Campus, Israel, February 25 – March 14.
17. ———, Georgia Institute of Technology Savannah, Georgia, USA, September 28 – October 7.
18. R. Henrion, Électricité de France R&D, Clamart, France, November 26–29.
19. D. Hömberg, University of Tokyo, Department of Mathematical Sciences, Japan, February 20 – March 3.
20. ———, Università degli Studi di Milano, Dipartimento di Matematica, Italy, March 19–30.
21. ———, University of Oxford, Mathematical Institute, UK, September 4 – December 20.
22. D. Horn, ALSTOM Power, Baden, Switzerland, August 20–24.
23. D. Kern, University of Oxford, Mathematical Institute, UK, October 1–5.
24. A. Kolodko, The University of Melbourne, Department of Mathematics and Statistics, Australia, January 29 – March 30.
25. ———, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, July 30 – August 15.
26. Ch. Kraus, Universität Freiburg, Abteilung für Angewandte Mathematik, December 10–15.
27. P. Krejčí, University of Tokyo, Graduate School of Mathematical Sciences, Japan, December 1–8.
28. P. Mathé, Vietnamese Academy of Science and Technology, Institute of Mathematics, Hanoi, July 2–12.
29. ———, Technische Universität Chemnitz, Fakultät für Mathematik, September 24–28.
30. ———, Austrian Academy of Sciences, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, October 31 – November 18.
31. A. Mielke, Istituto di Matematica Applicata e Tecnologie Informatiche — Consiglio Nazionale delle Ricerche, Pavia, Italy, November 18–22.
32. M. Pietrzyk, Universidade de Vigo, Facultade de Ciencias de Ourense, Area de Optica, Spain, June 30 – July 13.
33. J. Polzehl, University of Minnesota, School of Statistics, College of Liberal Arts, USA, May 18 – June 9.

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

34. M. RADZIUNAS, Departament de Fisica, Universitat de les Illes Balears, Palma de Mallorca, Spain, May 9–16.
35. O. ROTT, University of Oxford, Mathematical Institute, UK, November 5–9.
36. K.K. SABELFELD, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, January 2–28.
37. ———, Russian Academy of Sciences, Institute for Mathematical Modelling, Moscow, January 29 – February 2.
38. ———, Russian Academy of Sciences, Institute for Mathematical Modelling, Moscow, Russia, May 12–19.
39. ———, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, July 2 – August 12.
40. G. SCHMIDT, University of Liverpool, Department of Mathematical Sciences, UK, December 3–12.
41. V. SPOKOINY, Université de Rennes I, Institut de Recherche Mathématique de Rennes, France, March 5–16.
42. ———, National University of Singapore, Department of Statistics and Applied Probability, September 2–28.
43. H. STEPHAN, B. Verkin Institute for Low Temperature Physics and Engineering, Mathematical Division, Kharkov, Ukraine, July 3–7.
44. K. TABELOW, Cornell University, Weill Medical College, New York, USA, June 15–20.
45. A. VLADIMIROV, Ben Gurion University of the Negev, Department of Applied Mathematics, Beer-Sheva, Israel, April 16 – May 2.
46. V. WACHTEL, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, February 1–15.
47. W. WAGNER, Cambridge University, Centre for Mathematical Sciences and Department of Chemical Engineering, UK, May 8 – June 8.
48. M. WOLFRUM, University of Minnesota, School of Mathematics, Minneapolis, USA, March 3–16.
49. X. YAO, EURANDOM, Eindhoven, The Netherlands, March 18–24.

A.10 Academic Teaching[5]

Winter Semester 2006/2007

1. U. Bandelow, *Mechanik und Wärmelehre* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
2. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS.
3. A. Bovier, *Wahrscheinlichkeitstheorie II – BMS Basic Course Stochastic Processes I* (lecture), Technische Universität Berlin, 4 SWS.
4. 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.
5. W. Dreyer, *Projekt Nichtlineare Kontinuumsmechanik* (lecture), Technische Universität Berlin, Institut für Mechanik, 4 SWS.
6. A. Glitzky, *Optimale Steuerung bei parabolischen Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
7. R. Henrion, W. Römisch, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
8. E. Holzbecher, *Grundwassermodellierung II* (lecture), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
9. ———, *Grundwassermodellierung II* (practice), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
10. D. Hömberg, *Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
11. J. Kampen, *Nonstandard Stochastische Analysis (mit Anwendungen auf die Finanzmathematik)* (lecture), Ruprecht-Karls-Universität Heidelberg, 2 SWS.
12. A. Mielke, *Glattheit von Lösungen elliptischer Gleichungen und Variationsproblemen* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
13. H. Gajewski, B. Niethammer, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS.
14. J.G.M. Schoenmakers, *Einführung in die Stochastische Finanzmathematik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
15. V. Spokoiny, *Nichtparametrische Methoden und ihre Anwendungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
16. V. Spokoiny, W. Härdle, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
17. 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.
18. H. Stephan, *Konvexe Analysis* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
19. K. Tabelow, *Mathematik und Elektrotechnik* (seminar), Deutsches Herzzentrum Berlin, Akademie für Kardiotechnik, 4 SWS.
20. M. Wolfrum, J. Härterich, *Nichtlineare Dynamik* (senior seminar), WIAS/Freie Universität Berlin, 2 SWS.

Summer Semester 2007

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* (seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS.

[5] SWS = semester periods per week

3. D. Belomestny, *Advanced Methods in Quantitative Finance* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
4. M. Birkner, *Stochastische Modelle aus der Populationsbiologie* (lecture), Technische Universität Berlin, 2 SWS.
5. ———, *Stochastische Modelle aus der Populationsbiologie* (practice), Technische Universität Berlin, 1 SWS.
6. A. Bovier, *Wahrscheinlichkeitstheorie III – BMS Basic Course Stochastic Processes II* (lecture), Technische Universität Berlin, 4 SWS.
7. A. Bovier, H. Föllmer, P. Imkeller, U. Küchler, J.-D. Deuschel, J. Gärtner, M. Scheutzow, A. Schied, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS, 2 SWS.
8. A. Bovier, P. Ferrari, *Markov Processes and Applications* (seminar), Technische Universität Berlin, 2 SWS.
9. P. Gapeev, *Credit Risk: Modeling, Management and Valuation* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
10. J.A. Griepentrog, *Evolutionsgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
11. R. Henrion, *Optimierungsprobleme mit Zufallsrestriktionen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
12. R. Henrion, W. Römisch, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
13. E. Holzbecher, *Grundwassermodellierung I* (lecture), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
14. ———, *Grundwassermodellierung I* (practice), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
15. D. Hömberg, *Analysis für Ingenieure I* (lecture), Technische Universität Berlin, 4 SWS.
16. A. Mielke, D. Knees, *Variationsrechnung* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
17. ———, *Variationsrechnung* (practice), Humboldt-Universität zu Berlin, 2 SWS.
18. H. Gajewski, B. Niethammer, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS.
19. P. Philip, *Optimale Steuerung partieller Differentialgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
20. J.G.M. Schoenmakers, *Stochastische Finanzmathematik II* (lecture), Humboldt-Universität zu Berlin, 3 SWS.
21. V. Spokoiny, *Moderne Methoden in der nichtparametrischen Statistik* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
22. V. Spokoiny, W. Härdle, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
23. 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.
24. H. Stephan, *Mathematische Modellierung* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
25. K. Tabelow, *Mathematik und Elektrotechnik* (seminar), Deutsches Herzzentrum Berlin, Akademie für Kardiotechnik, 4 SWS.
26. M. Wolfrum, J. Härterich, *Nichtlineare Dynamik* (senior seminar), WIAS/Freie Universität Berlin, 2 SWS.

Winter Semester 2007/2008

1. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (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.

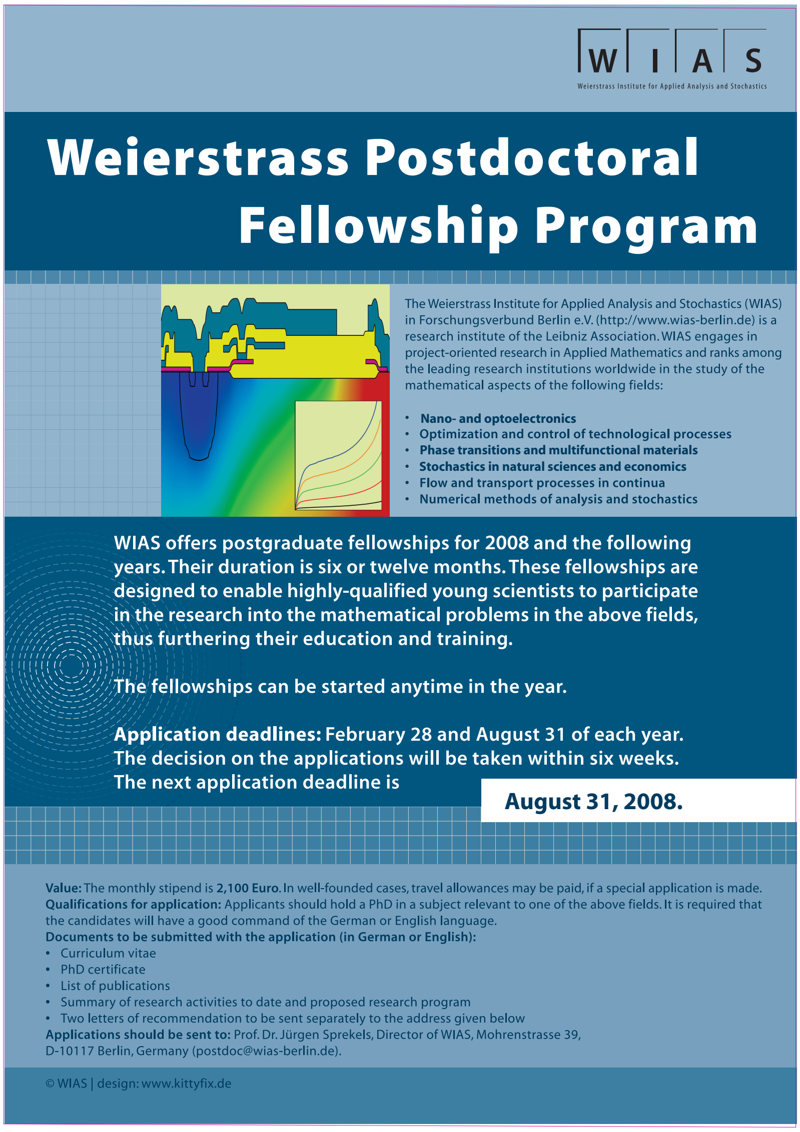
4. ———, *Oberseminar biologische Modelle und statistische Mechanik* (senior seminar), Technische Universität Berlin, 2 SWS.
5. A. Bovier, H. Föllmer, P. Imkeller, U. Küchler, J.-D. Deuschel, J. Gärtner, M. Scheutzow, A. Schied, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
6. W. Dreyer, *Tensoranalysis* (lecture), Technische Universität Berlin, Institut für Mechanik, 4 SWS.
7. P. Ferrari, *Random Matrices and Related Problems* (lecture), Technische Universität Berlin, 3 SWS.
8. A. Glitzky, *Einführung in die Kontrolltheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
9. J.A. Griepentrog, *Funktionenräume 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, *Grundwassermodellierung II* (lecture), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
13. ———, *Grundwassermodellierung II* (practice), Freie Universität Berlin, Fachbereich Geowissenschaften, 1 SWS.
14. D. Hömberg, *Optimal Control of Partial Differential Equations (Michaelmas Term 2007)* (lecture), University of Oxford, 2 SWS.
15. Ch. Meyer, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
16. A. Mielke, *Ausgewählte Themen der Variationsrechnung* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
17. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS.
18. V. Spokoiny, *Nichtparametrische Methoden und ihre Anwendungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
19. V. Spokoiny, W. Härdle, *Mathematische Statistik* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
20. J. Sprekels, *Höhere Analysis I (Funktionalanalysis)/BMS Basic Course "Functional Analysis"* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
21. 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.
22. K. Tabelow, *Mathematik und Elektrotechnik* (seminar), Deutsches Herzzentrum Berlin, Akademie für Kardiotechnik, 4 SWS.
23. M. Wolfrum, S. Liebscher, *Nichtlineare Dynamik* (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 2007, Dr. Giada Basile (Université de Paris-Dauphine, France, and Università degli Studi di Firenze, Italy), Dr. Michela Eleuteri (Università degli Studi di Trento, Italy), Dr. Robert Haller-Dintelmann (Technische Universität Darmstadt), Dr. Xin Yao (Tsinghua University, Beijing, China), and Dr. Olivier Zindy (Université Paris VI, France) have worked as fellowship holders at WIAS.



A.12 Visiting Scientists[6]

A.12.1 Guests

1. G. Bao, Michigan State University, Department of Mathematics, East Lansing, USA, July 26–31.
2. Y. Baraud, Université de Nice Sophia-Antipolis, Laboratoire J. A. Dieudonné, France, June 19–22.
3. N. Berglund, CNRS Centre de Physique Théorique, Marseille, and Université de Toulon et du Var, Physique Mathématique Théorique, Toulon, France, April 16–21.
4. A.B. Bhattacharjee, Max-Planck-Institut für Physik komplexer Systeme, Dresden, October 12–21.
5. A. Bradji, Berlin, March 1 – April 9.
6. M. Brokate, Technische Universität München, Zentrum Mathematik, October 29 – November 2.
7. F. Cagnetti, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, September 16–21.
8. N. Champagnat, INRIA — Sophia Antipolis, France, May 17–26.
9. K. Chełminski, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, June 18 – July 11.
10. R. Ciegis, Vilnius Gediminas Technical University, Department of Mathematics, Lithuania, November 2–30.
11. P. Cizek, Tilburg University, Department of Econometrics and Operations Research, The Netherlands, May 6–11.
12. P. Cook, University of Delaware, Department of Mathematical Sciences, Newark, USA, August 26 – September 8.
13. J.C. de los Reyes, Escuela Politécnica Nacional, Quito, Departamento de Matemática, Ecuador, September 2–30.
14. A. Dressel, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, October 21–26.
15. J. Einmahl, Tilburg University, Department of Econometrics and Operations Research, The Netherlands, November 12–15.
16. P. Evans, Humboldt-Universität zu Berlin, Institut für Mathematik, July 27, 2006 – December 31, 2009.
17. P. Exner, Academy of Sciences of the Czech Republic, Nuclear Physics Institute, Prague, February 12–28.
18. M. Falcone, Università di Roma “La Sapienza”, Dipartimento di Matematica, February 5–17.
19. E. Feireisl, Academy of Sciences of the Czech Republic, Mathematical Institute, Prague, November 12–23.
20. ———, December 3–7.
21. G. Francfort, Université Paris 13, Laboratoire des Propriétés Mécaniques et Thermodynamiques des Matériaux, Institut Galilée, Villetaneuse, France, March 29 – April 1.
22. A. Garroni, Università di Roma “La Sapienza”, Dipartimento di Matematica, Italy, March 29 – April 1.
23. A. Gaudilliere, Università Roma Tre, Dipartimento di Matematica, Italy, December 12–22.
24. J. Giannoulis, Technische Universität München, Zentrum Mathematik, August 14 – September 10.
25. A. Goldenshluger, University of Haifa, Department of Statistics, Israel, July 10–24.
26. Y. Golubev, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, May 3–31.
27. J. Habermann, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, July 30 – August 3.
28. D.N. Hào, Vietnamese Academy of Science and Technology, Institute of Mathematics, Hanoi, August 27–31.

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

29. B. Heubeck, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Informatik, November 18–23.
30. B. Hofmann, Technische Universität Chemnitz, Fakultät für Mathematik, March 12–16.
31. M. Huber, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, January 22–27.
32. D. Ioffe, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, July 15 – August 19.
33. J. Johannes, Universität Heidelberg, Institut für Angewandte Mathematik, May 14–18.
34. A. Juditsky, Université Joseph Fourier Grenoble I, Laboratoire de Modélisation et Calcul, France, October 27 – November 20.
35. Ch. Keul, RWTH Aachen, Institut für Eisenhüttenkunde, November 26–29.
36. D. Kourounis, University of Ioannina, Department of Material Science, Greece, September 19 – October 12.
37. M. Kraft, University of Cambridge, Department of Chemical Engineering, UK, August 20 – September 9.
38. R. Krämer, Technische Universität Chemnitz, Fakultät für Mathematik, August 13–17.
39. O. Kurbanmuradov, Turkmen State University, Physics and Mathematics Research Center, Ashkhabat, April 28 – June 28.
40. ———, October 2 – December 2.
41. A. Levykin, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, April 1 – May 1.
42. K. Löschner-Greenberg, Robert Bosch GmbH, CR/ARE3, Stuttgart, September 17–23.
43. M.M. Malamud, Donetsk National University, Department of Mathematics, Ukraine, November 21 – December 19.
44. M. Malioutov, Northeastern University, Department of Mathematics, Boston, USA, June 28 – July 12.
45. M. Mascagni, Florida State University, Department of Computer Science, Tallahassee, USA, December 7–12.
46. S. Mathew, Johann Wolfgang Goethe-Universität, Frankfurt am Main, October 8–12.
47. H. Mena, Technische Universität Chemnitz, Fakultät für Mathematik, September 27–30.
48. G.N. Milstein, Ural State University, Department of Mathematics, Ekaterinburg, Russia, April 1 – August 31.
49. A. Miranville, Université de Poitiers, Laboratoire d'Applications des Mathématiques, France, July 2–13.
50. ———, October 7–20.
51. M. Möhle, Heinrich-Heine-Universität Düsseldorf, Mathematisches Institut, October 2–5.
52. A. Münch, University of Nottingham, School of Mathematical Sciences, UK, September 1, 2007 – August 31, 2009.
53. O. Muscato, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, June 16–23.
54. P. Mykland, The University of Chicago, Department of Statistics, USA, July 16–21.
55. L. Mytnik, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, March 6–11.
56. F. Nardi, EURANDOM, Eindhoven, The Netherlands, December 15–19.
57. P. Neff, Technische Universität Darmstadt, Fachbereich Mathematik, August 27 – September 11.
58. F. Nier, Université de Rennes I, Institut de Recherche Mathématique de Rennes (IRMAR), France, July 15–22.
59. B. Niethammer, University of Oxford, Mathematical Institute, UK, December 17–22.
60. L. Paoli, Université de Saint-Etienne, Laboratoire de Mathématique, France, June 11–29.
61. V. Patilea, École Nationale de la Statistique et de l'Analyse de l'Information, Bruz, France, June 4–8.
62. A. Pimenov, University College Cork, School of Mathematical Sciences, Ireland, June 23 – July 4.

63. D. Rachinskii, University College Cork, School of Mathematical Sciences, Ireland, January 4–10.
64. ———, June 30 – July 16.
65. J. Rademacher, Centrum voor Wiskunde en Informatica, Department Modelling, Analysis and Simulation, Amsterdam, The Netherlands, January 13 – February 11.
66. P. Rigollet, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, July 3–21.
67. W. Ring, Karl-Franzens-Universität Graz, Institut für Mathematik, Austria, August 11 – September 3.
68. S. Rjasanow, Universität des Saarlandes, Fachrichtung Mathematik, August 27 – September 7.
69. E. Rocca, Università degli Studi di Milano, Dipartimento di Matematica "F. Enriques", Italy, August 27–31.
70. N. Rosanov, Vavilov State Optical Institute, Institute for Laser Physics, St. Petersburg, Russia, November 18–23.
71. P. Rosenau, Tel-Aviv University, School of Mathematics, Israel, June 4–19.
72. R. Rossi, Università degli Studi di Brescia, Dipartimento di Matematica, Italy, January 28–31.
73. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, September 6–16.
74. I. Rubinstein, Ben Gurion University of the Negev, Jacob Blaustein Institute for Desert Research, Sede Boqer Campus, Israel, August 1 – September 30.
75. O. Schenk, University of Basel, Department of Computer Science, Switzerland, October 15 – November 9.
76. N. Serdyukova, St. Petersburg State University, Department of Mathematics and Mechanics, Russia, November 15–22.
77. I. Shalimova, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, February 1 – March 1.
78. ———, March 8 – April 8.
79. ———, May 18 – June 18.
80. ———, October 15 – December 15.
81. Z. Shi, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, June 12–16.
82. J. Sieber, University of Aberdeen, School of Engineering, UK, December 14–21.
83. C. Spitoni, EURANDOM, Eindhoven, The Netherlands, February 25 – March 3.
84. ———, December 15–20.
85. C. Starica, Chalmers University of Technology, Department of Mathematical Statistics, Gothenburg, Sweden, March 2–8.
86. J. Stockie, Simon Fraser University, Department of Mathematics, Burnaby, Canada, October 31 – November 3.
87. N. Suciu, Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Angewandte Mathematik, November 19 – December 2.
88. P. Tankov, Université Paris VII, Laboratoire de Probabilités et Modèles Aléatoires, France, June 18–29.
89. D. Tiba, Romanian Academy, Institute of Mathematics, Bucharest, September 17 – October 12.
90. M. Tretyakov, University of Leicester, Department of Mathematics, UK, July 1–31.
91. D. Turaev, Ben Gurion University of the Negev, Department of Mathematics, Beer Sheva, Israel, July 19 – August 5.
92. ———, October 3–15.
93. S. van Bellegem, Université Catholique de Louvain, Institut de Statistique, Louvain-la-Neuve, Belgium, January 14–18.
94. C. Vial, Université Paris X, Laboratoire Modal'X, Nanterre, France, April 23–28.
95. E. Viktorov, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, December 10–14.
96. H. Voss, Cornell University, Weill Medical College, New York, USA, May 7–16.

97. J. Xiong, Guangzhou University, School of Mathematics and Information Science, China, January 15 – February 12.
98. M. Yamamoto, University of Tokyo, Department of Mathematical Sciences, Japan, March 26 – April 23.
99. B. Zaltzman, Ben Gurion University of the Negev, Jacob Blaustein Institute for Desert Research, Sede Boqer Campus, Israel, September 12–28.
100. Ch. Zanini, Ecole Polytechnique, Centre de Mathématiques Appliquées (CMAP), Palaiseau, France, March 18 – April 30.
101. S. Zelik, University of Surrey, Department of Mathematics, Guildford, UK, November 26 – December 22.
102. O. Zindy, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, July 7–14.

A.12.2 Scholarship Holders

1. G. Basile, Université de Paris-Dauphine, France, and Università degli Studi di Firenze, Italy, Weierstrass Postdoctoral Fellowship Program, September 1, 2007 – August 31, 2008.
2. M. Eleuteri, Università degli Studi di Trento, Dipartimento di Matematica, Italy, Weierstrass Postdoctoral Fellowship Program, January 1 – December 31.
3. R. Haller-Dintelmann, Technische Universität Darmstadt, Fachbereich Mathematik, Weierstrass Postdoctoral Fellowship Program, October 1, 2006 – September 30, 2007.
4. A. Levykin, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, Russia, DAAD Fellowship, October 4 – December 4.
5. M. Luczak, London School of Economics, Department of Mathematics, Humboldt Research Fellowship, November 1 – December 31.
6. A. Münch, Humboldt-Universität zu Berlin, Institut für Mathematik, Heisenberg Fellowship of the Deutsche Forschungsgemeinschaft (German Research Foundation), November 1, 2003 – August 31, 2007.
7. L. Panizzi, Scuola Normale Superiore, Pisa, Italy, Postdoctoral Fellowship of the Scuola Normale Superiore, March 9, 2006 – April 9, 2007.
8. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, Humboldt Research Fellowship, January 15 – February 15.
9. X. Yao, Tsinghua University, Department of Automation, Beijing, PR China, Weierstrass Postdoctoral Fellowship Program, March 1, 2006 – March 31, 2007.
10. 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, since January 1, 2004.
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. S. Hock, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", doctoral candidate, May 1, 2005 – December 31, 2008.
4. S.-J. Kimmerle, Humboldt-Universität zu Berlin, Institut für Mathematik, DFG Research Center Matheon, subproject C14, doctoral candidate, January 1, 2007 – May 31, 2010.
5. 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.
6. A. Klimovski, Technische Universität Berlin, doctoral candidate, since June 1, 2003.
7. 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.

8. 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, 2008.
9. 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.
10. 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, 2008.
11. 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. R. Abeyaratne, Massachusetts Institute of Technology, Department of Mechanical Engineering, Cambridge, USA, *Atomistic to continuum modeling of the motion of material interfaces*, July 17.
2. G. Bao, Michigan State University, Department of Mathematics, East Lansing, USA, *Recent developments for inverse problems in electromagnetic wave propagation*, July 27.
3. Y. Baraud, Université de Nice Sophia-Antipolis, Laboratoire J.A. Dieudonné, France, *Gaussian model selection when the variance is unknown*, June 20.
4. J. Behrndt, Technische Universität Berlin, Institut für Mathematik, *Boundary value problems for elliptic partial differential operators on bounded domains*, January 30.
5. N. Berglund, CNRS Centre de Physique Théorique, Marseille, and Université de Toulon et du Var, Physique Mathématique Théorique, Toulon, France, *Metastability in a chain of coupled nonliner diffusions*, April 18.
6. A.B. Bhattacharjee, Max-Planck-Institut für Physik komplexer Systeme, Dresden, *Bose–Einstein condensates in optical lattices*, October 18.
7. F. Cagnetti, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, *A vanishing viscosity approach to fracture growth in a cohesive zone model with prescribed crack path*, September 19.
8. N. Champagnat, INRIA — Sophia Antipolis, France, *A microscopic interpretation of evolutionary branching: The limit of rare mutations in a stochastic model of evolution with logistic interaction*, May 23.
9. K. Chełminski, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, *On a nonmonotone flow rule in the inelastic deformation theory*, July 3.
10. R. Ciegis, Vilnius Gediminas Technical University, Department of Mathematical Modeling, Lithuania, *Analysis of upwind and high-resolution schemes for solving convection dominated problems in porous media*, November 29.
11. P. Cook, University of Delaware, Department of Mathematical Sciences, Newark, USA, *Modeling of complex fluids; the inhomogeneous response in steady and transient flows of wormlike micellar solutions*, August 31.
12. J.C. de los Reyes, Escuela Politécnica Nacional, Quito, Departamento de Matemática, Ecuador, *Boundary flow control with pointwise state-constraints*, September 11.
13. E. Dintelmann, Technische Universität Darmstadt, Fachbereich Mathematik, *L^p theory for fluids around moving obstacles*, July 25.
14. M. Ehrhardt, Technische Universität Berlin, Institut für Mathematik, *A review of transparent and artificial boundary conditions techniques for linear and nonlinear Schrödinger equations*, July 4.
15. J. Einmahl, Tilburg University, Department of Econometrics and Operations Research, The Netherlands, *Asymptotics for the Hirsch index*, November 14.
16. ———, *Records in athletics through extreme-value theory*, November 14.
17. M. Eleuteri, Università degli Studi di Trento, Dipartimento di Matematica, Italy, *An introduction to direct methods in the calculus of variations and some recent regularity results*, March 13.
18. P. Exner, Academy of Sciences of the Czech Republic, Nuclear Physics Institute, Prague, *Usual ways to decay*, February 20.
19. ———, *Geometrically induced spectral properties of quantum layers*, February 21.
20. M. Falcone, Università di Roma "La Sapienza", Dipartimento di Matematica, Matheon *Special Guest Lecture: An introduction to viscosity solutions – Theory, numerics and applications*, February 7.
21. ———, Matheon *Special Guest Lecture: An introduction to viscosity solutions – Theory, numerics and applications: Approximation schemes for viscosity solutions*, February 7.
22. ———, Matheon *Special Guest Lecture: An introduction to viscosity solutions – Theory, numerics and applications: Image processing*, February 14.
23. ———, Matheon *Special Guest Lecture: An introduction to viscosity solutions –Theory, numerics and applications: Control problems*, February 14.

24. R. Farwig, Technische Universität Darmstadt, Fachbereich Mathematik, *Strömungen um rotierende Hindernisse: Grundlegende Fragestellungen und überraschende Ergebnisse*, January 17.
25. E. Feireisl, Academy of Sciences of the Czech Republic, Mathematical Institute, Prague, *On a diffuse interface model for a two-phase flow of compressible viscous fluids*, November 21.
26. B. Fiedler, Freie Universität Berlin, Fachbereich Mathematik und Informatik, *Design of planar global attractors of Sturm type*, July 11.
27. J. Giannoulis, Technische Universität München, Zentrum Mathematik, *Reduced Hamiltonian structures for interacting pulses in nonlinear lattices*, August 22.
28. M. Giehler, Paul-Drude-Institut für Festkörperelektronik, Berlin, *Optische Moden von Zweisektions-Quantenkaskadenlasern für den mittleren-infraroten und Terahertz Spektralbereich*, February 8.
29. A. Goldenshluger, University of Haifa, Department of Statistics, Israel, *A universal procedure for aggregating estimators*, July 11.
30. Y. Golubev, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, *On m-spacing entropy estimators for vanishing densities*, May 30.
31. B.K. Goswami, Bhabha Atomic Research Centre, Mumbai, India, *Self-similarity in multistability — A possible universal feature*, October 25.
32. A. Gual i Coca, Heinrich-Hertz-Institut für Nachrichtentechnik, Berlin, *Wellenlängenumsetzungen in passiven Wellenleiterstrukturen*, June 7.
33. J. Habermann, Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematisches Institut, *An introduction to regularity theory for variational problems with non-standard growth*, July 31.
34. C. Hager, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, *Numerische Methoden für die Simulation von zeitabhängigen Kontaktproblemen*, January 23.
35. R. Haller-Dintelmann, Technische Universität Darmstadt, Fachbereich Mathematik, *Square roots of divergence form operators*, March 21.
36. ———, *Irreducibility and mixed boundary conditions*, April 18.
37. ———, *Maximale Regularität für Divergenzform-Operatoren auf Sobolev-Räumen*, November 28.
38. K. Hermsdörfer, Albert-Ludwigs-Universität Freiburg, Abteilung für Angewandte Mathematik, *The pressure interface condition across phase boundaries*, August 21.
39. B. Heubeck, Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Informatik, *A new simulation technique for the optical wave in distributed feedback lasers*, November 22.
40. M. Hieber, Technische Universität Darmstadt, Fachbereich Mathematik, *Die Navier-Stokes-Gleichungen und rotierende Fluide*, January 24.
41. B. Hofmann, Technische Universität Chemnitz, Fakultät für Mathematik, *Nature of ill-posedness and regularization of some nonlinear inverse problems in option pricing*, March 13.
42. M. Huber, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, *Simulation of diffraction on periodic media with a coupled finite element and plane wave approach*, January 23.
43. J. Johannes, Universität Heidelberg, Institut für Angewandte Mathematik, *Deconvolution with unknown error distribution*, May 16.
44. A. Juditsky, Université Joseph Fourier Grenoble I, Laboratoire de Modélisation et Calcul, France, *Nonparametric estimation by convex programming*, November 6.
45. S.A. Kashenko, Yaroslavl State University, Department of Mathematical Modeling, Russia, *Asymptotic methods for laser equations with delayed feedback*, March 15.
46. H.P. Kavehpour, University of California, Department of Mechanical & Aerospace Engineering, Los Angeles, USA, *Coalescence of liquid drops: Physics, challenges and bouncelets*, February 6.
47. Ch. Keul, RWTH Aachen, Institut für Eisenhüttenkunde, *Beschreibung der Phasenumwandlung in Stählen mittels Dilatometrie*, November 27.
48. B.N. Khoromskij, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Tensor-product approximation in $\mathbb{R}^d$ with applications to electronic structure calculations*, July 10.
49. S.-J. Kimmerle, Humboldt-Universität zu Berlin, Institut für Mathematik, *A macroscopical model for precipitation in GaAs crystals*, May 8.

50. E.R. KOCHAROVSKAYA, Russian Academy of Sciences, Institute of Applied Physics, Nizhny Novgorod, *Superradiant lasing in photonic crystals*, June 26.
51. V.V. KOCHAROVSKY, Russian Academy of Sciences, Institute of Applied Physics, Nizhny Novgorod, *Dual-wavelength semiconductor lasers and intracavity mode mixing in CW and mode-locking regimes*, June 26.
52. M. KRAFT, University of Cambridge, Department of Chemical Engineering, UK, *Particle processes: Characterisation from micro scale to macro scale*, September 5.
53. A. KRAWIETZ, Technische Fachhochschule Berlin, Fachbereich Maschinenbau, Verfahrens- & Umwelttechnik, *Kontinuumsmechanik von Tensidfilmen und Mikroemulsionen*, November 13.
54. K. KRISCHER, Technische Universität München, Physik-Department E19, *Dynamic instabilities in fuel cell relevant reactions*, September 20.
55. C. KRÜGER, Berlin, *Exact operator quantization of the Euclidean black hole CFT*, July 12.
56. O. KURBANMURADOV, Turkmen State University, Physics and Mathematics Research Center, Ashkhabat, *Randomized spectral and Fourier-wavelet models for simulation of random fields*, November 20.
57. S. LIEBSCHER, Brown University, Division of Applied Mathematics, Providence, USA, *Bifurcations without parameter in PDEs*, January 16.
58. K. LÖSCHNER-GREENBERG, Robert Bosch GmbH, CR/ARE3, Stuttgart, *A new vector Preisach operator for modeling magnetic hysteresis*, September 18.
59. M. LÖWE, Westfälische Wilhelms-Universität Münster, Institut für Mathematische Statistik, *The swapping algorithm for the random field Curie–Weiss model*, June 20.
60. M. LUCZAK, London School of Economics, *Quantitative laws of large numbers for Markov processes in countably many dimensions*, December 12.
61. M.M. MALAMUD, Donetsk National University, Department of Mathematics, Ukraine, *Elliptic boundary value problems*, December 12.
62. M. MALIOUTOV, Northeastern University, Department of Mathematics, Boston, USA, *Statistical discrimination and universal compressors*, July 10.
63. M. MASCAGNI, Florida State University, Department of Computer Science, Tallahassee, USA, *Novel stochastic methods in biochemical electrostatics*, December 11.
64. S. MEIER, Universität Bremen, Zentrum für Technomathematik, *A two-scale reaction-diffusion system with evolving microstructure*, January 31.
65. H. MENA, Technische Universität Chemnitz, Fakultät für Mathematik, *Numerical solution of differential Riccati equations arising in optimal control problems*, September 28.
66. B. MICHEL, Simuloptics GmbH Schwabach, *Inverses Streuproblem bei der optischen Partikelcharakterisierung*, November 26.
67. A. MIRANVILLE, Université de Poitiers, Laboratoire d'Applications des Mathématiques, France, *Asymptotic behavior of some triply nonlinear equations*, July 10.
68. ———, *The Cahn–Hilliard equation with dynamic boundary conditions*, October 17.
69. P. MYKLAND, The University of Chicago, Department of Statistics, USA, *Locally parametric inference in high frequency data*, July 18.
70. P. NEFF, Technische Universität Darmstadt, Fachbereich Mathematik, *Minimale Cosserat-Rotationen und synthetische Reproduktion einer Nano-Einkerbung*, August 28.
71. ———, *Notes on strain gradient plasticity: Finite strain covariant modelling and global existence in the infinitesimal rate-independent case*, September 5.
72. F. NIER, Université de Rennes I, Institut de Recherche Mathématique de Rennes (IRMAR), France, *Accurate WKB approximation for a 1D problem with low regularity*, July 18.
73. B. NIETHAMMER, University of Oxford, Mathematical Institute, UK, *On the effect of encounters in domain coarsening*, December 18.
74. F. OTTO, Universität Bonn, Institut für Angewandte Mathematik, *Coarsening and energy landscapes*, July 6.
75. L. PAOLI, Université de Saint-Etienne, Laboratoire de Mathématique, France, *Asymptotics for some vibro-impact problems with a linear dissipation term*, June 13.

76. V. Patilea, École Nationale de la Statistique et de l'Analyse de l'Information, Bruz, France, *Nonparametric lack-of-fit tests for parametric mean-regression models with censored data*, June 6.
77. M.A. Peter, Universität Bremen, Zentrum für Technomathematik, *Homogenisation of coupled reaction-diffusion systems in porous media with evolving microstructure*, April 25.
78. J. Rademacher, Centrum foor Wiskunde en Informatica, Department Modelling, Analysis and Simulation, Amsterdam, The Netherlands, *Dispersive and non-classical shocks in the hyperbolic continuum limit of FPU chains*, November 6.
79. L. Recke, Humboldt-Universität zu Berlin, Institut für Mathematik, *A new implicit function theorem and applications to singularly perturbed boundary value problems*, May 16.
80. P. Rigollet, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, *Stochastic optimization using mirror averaging algorithm. Application to classification and other statistical problems*, July 4.
81. W. Ring, Karl-Franzens-Universität Graz, Institut für Mathematik, Austria, *Geometric ideas for the solution of state-constrained optimal control problems*, August 21.
82. E. Rocca, Università degli Studi di Milano, Dipartimento di Matematica "F. Enriques", Italy, *Analysis of a nonlinear degenerating PDE system for phase transitions in thermoviscoelastic materials*, August 29.
83. R. Rossi, Università degli Studi di Brescia, Dipartimento di Matematica, Italy, *Long-time behaviour of gradient flows in metric spaces*, January 31.
84. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, *Gradient estimates for heat equation with L1-data and applications to thermomechanical systems*, February 7.
85. ———, *Rate-independent processes in viscous solids and their thermodynamics*, September 12.
86. I. Rubinstein, Ben Gurion University of the Negev, Jacob Blaustein Institute for Desert Research, Sede Boqer Campus, Israel, *Bulk electroconvective instability*, September 19.
87. O. Schenk, University of Basel, Department of Computer Science, Switzerland, *General-purpose sparse matrix building blocks on Graphics Processing Units*, October 25.
88. A. Schlömerkemper, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *A multi-scale analysis of magnetic forces between rigid bodies*, May 2.
89. S. Schwertfeger, Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin, *Mode locking with 4 sections DBR laser*, January 25.
90. N. Serdyukova, St. Petersburg State University, Department of Mathematics and Mechanics, Russia, *Intractability rate of approximation problem for random fields in increasing dimension*, November 20.
91. I. Shalimova, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, *Stochastic simulation method for solving elasticity problem with random loads*, February 27.
92. Z. Shi, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, *Random walk, polymer, tree*, June 13.
93. A. Shilnikov, Georgia State University, Department of Mathematics and Statistics, Atlanta, USA, *Complex homoclinic bifurcations in slow-fast neuronal models*, October 30.
94. J. Sieber, University of Aberdeen, School of Engineering, UK, *Continuation with feedback control: First results from mechanical experiments*, December 20.
95. M. Spreemann, Humboldt-Universität zu Berlin, Institut für Physik, *Nonlinear effects in lasers with tapered sections*, January 11.
96. I. Steinbach, ACCESS e. V., Aachen, *Influence of lattice strain on the transformation kinetics of pearlite*, October 30.
97. M. Steinbach, Leibniz Universität Hannover, *Optimierungsalgorithmen zur Betriebsplanung in Wasser- und Gasnetzen*, April 3.
98. J. Stockie, Simon Fraser University, Department of Mathematics, Burnaby, Canada, *Multiscale modelling of the fuel cell catalyst layer*, November 1.
99. H. Struchtrup, University of Victoria, Department of Mechanical Engineering, Canada, *Models for non-equilibrium evaporation and condensation*, October 30.

100. P. Tankov, Université Paris VII, Laboratoire de Probabilités et Modèles Aléatoires, France, *Constant proportion portfolio insurance in presence of jumps in asset prices*, June 19.
101. D. Tiba, Romanian Academy, Institute of Mathematics, Bucharest, *Optimal control methods in shape optimization*, September 25.
102. E.S. Titi, University of California, Department of Mathematics, Irvine, USA, *Global regularity for three-dimensional Navier–Stokes equations and other relevant geophysical models*, December 5.
103. M. Tretyakov, University of Leicester, Department of Mathematics, UK, *Computing ergodic limits for Langevin equation*, July 3.
104. D. Turaev, Ben Gurion University of the Negev, Department of Mathematics, Beer Sheva, Israel, *Unbounded energy growth in non-autonomous Hamiltonian systems*, July 31.
105. O. Ushakov, Humboldt-Universität zu Berlin, Institut für Physik, *Excitability of chaotic transients in a semiconductor laser*, February 1.
106. S. van Bellegem, Université Catholique de Louvain, Institut de Statistique, Louvain-la-Neuve, Belgium, *Inference in semi- and nonparametric regression with instrumental variables*, January 17.
107. M. Väth, Freie Universität Berlin, Institut für Informatik, *Bifurcation of reaction-diffusion systems with inclusions in the stable domain*, January 9.
108. S. Vigerske, Humboldt-Universität zu Berlin, Institut für Mathematik, *LaGO — Branch and Cut für nichtkonvexe MINILPs*, January 30.
109. E.A. Viktorov, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, *Modelocking in quantum dash lasers*, December 13.
110. J. Villain, Fachhochschule Augsburg, FB Elektrotechnik, *Struktur und Eigenschaften miniaturisierter bleifreier Lötverbindungen*, October 29.
111. P. Vogl, Technische Universität München, Walter-Schottky-Institut, *The 3D nanometer device project nextnano: Concepts, methods, results*, November 26.
112. H. Voss, Cornell University, Weill Medical College, New York, USA, *Imaging neuronal connectivity*, May 15.
113. D. Wegner, Humboldt-Universität zu Berlin, Institut für Mathematik, *Zur Existenz von Lösungen eines lokalen Phasenfeldmodells der Phasentrennung*, February 20.
114. M. Welk, Universität des Saarlands, Fakultät für Mathematik und Informatik, *Robust variational methods for the deconvolution of images*, December 17.
115. H. Wenzel, Ferdinand-Braun-Institut für Höchstfrequenztechnik Berlin, *High-brightness diode lasers — Achievements and challenges*, October 29.
116. M. Wilke, Martin-Luther-Universität Halle-Wittenberg, Institut für Mathematik, *Maximal L^p regularity for the Cahn–Hilliard–Gurtin equations and long-time behavior*, December 19.
117. C. Wolters, Westfälische Wilhelms-Universität Münster, Institut für Biomagnetismus und Biosignalanalyse, *Numerical approaches for finite element method based EEG and MEG source analysis*, February 12.
118. U. Wulf, Brandenburgische Technische Universität Cottbus, Lehrstuhl Theoretische Physik, *Multi-saddle-point approximation for pulse propagation in resonant tunneling*, March 6.
119. M. Yamamoto, University of Tokyo, Department of Mathematical Sciences, Japan, *Tikhonov discretized regularization by using reproducing kernel Hilbert spaces*, April 20.
120. B. Zaltzman, Ben Gurion University of the Negev, Jacob Blaustein Institute for Desert Research, Sede Boqer Campus, Israel, *Electroosmotic flows and electroconvection – From theory to experiment*, September 20.
121. Ch. Zanini, Ecole Polytechnique, Centre de Mathématiques Appliquées (CMAP), Palaiseau, France, *Quasistatic crack growth for a cohesive zone model with prescribed crack*, March 23.
122. S. Zelik, University of Surrey, Department of Mathematics, Guildford, UK, *Chaotic soliton interaction and space-time chaos in 1D Ginzburg–Landau equations*, December 4.

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: 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 mainly by using adaptive methods of cluster analysis, classification, and multivariate visualization. The main focus here is on simple stable models accompanied by appropriate multivariate (graphical) methods like principal components plots and informative dendrograms (binary trees). Usually, the performance and stability of these methods can be improved by using them in a local and adaptive local fashion. However, the main focus is on clustering techniques. A highlight is the automatic validation technique of cluster analysis results performed by a general built-in validation tool that is based on resampling techniques. 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, such as the adjusted Rand index. Second, the stability of each individual cluster is assessed based on measures of similarity between sets, e.g., the asymmetric measure of cluster agreement or the symmetric Jaccard measure. It does makes sense to investigate the (often quite different) specific stability of clusters. In the third and most detailed level of validation, the reliability of the cluster membership of each individual observation can be assessed.

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`.

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, it 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 3D 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 3D 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 intense heating by induction. The simulator accounts for heat transfer by radiation through cavities, and it allows for changes in the material parameters due to the rising temperature and for some kinds of anisotropy within the thermal conductivity. 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 2D projection. The software is based on the WIAS program package pdelib for the numerical solution of partial differential equations and has a graphical user interface provided by WIAS-MatConE.

WIAS-HiTNIHS 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, 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 adaptive grid is used. To facilitate its usage, a Java-based GUI has been developed.

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

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

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

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

WIAS-QW (contact: 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`.