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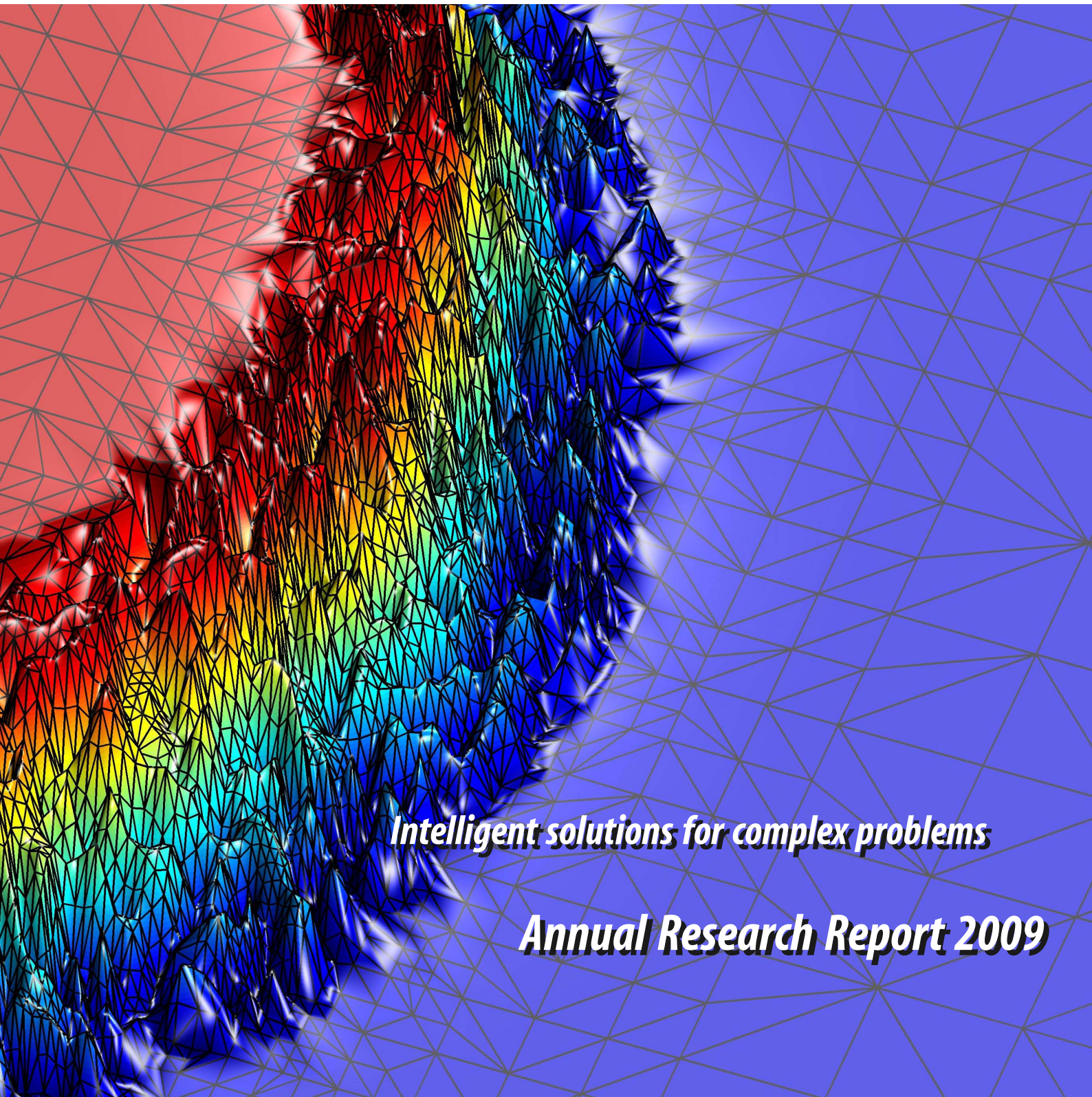
Weierstrass Institute for Applied Analysis and Stochastics



Intelligent solutions for complex problems

Annual Research Report 2009

Cover figure: Finite Element simulation of phase separation phenomena in metal alloys where the initial configuration is perturbed with random noise.

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The Weierstrass Institute for Applied Analysis and Stochastics (WIAS, member of the Leibniz Association) presents its Annual Report 2009. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2009. Following a more general introduction in part one, in its second part seven selected scientific contributions, written for a broader public, highlight some results of outstanding importance. Finally, the third part presents the essential results of the research groups.

Prof. Dr. Jürgen Sprekels, Director

The year 2009 was marked by continuing last year's successful work in the *Research Program 2007–2009*. WIAS further consolidated its leading position in the mathematical community as a center of excellence in the treatment of complex applied problems. Several scientific breakthroughs were achieved, some of which will be detailed later in this report, and WIAS has further expanded its scope into new applied problems from medicine, economy, science, and engineering, especially in its main application areas:

- Nano- and optoelectronics
- Optimization and control of technological processes
- Phase transitions and multifunctional materials
- Flow and transport processes in continua
- Random phenomena in nature and economy

Besides the international workshops organized by the institute, the 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's positive development is best reflected by the acquisition of grants: the best result ever was achieved. Altogether, 37 additional co-workers could be financed from these grants.

The institute's years-long success in the acquisition of grants became visible in the "Funding Ranking 2009" of the German Research Foundation DFG: in the years 2005–2007, WIAS acquired the largest DFG funding in the field of mathematics among all non-university research institutions in Germany.

In addition to this, WIAS took part in two successful applications within the Excellence Competition of the Leibniz Association in 2009, namely the projects "ECONS: Evolving Complex Networks – Regionales Ressourcen-Management unter den Bedingungen des Umwelt- und demografischen Wandels" (Regional resource management under the conditions of environmental and demographic change, headed by the Potsdam Institute for Climate Impact Research, PIK) and „Multiplizität, Modellvalidierung und Reproduzierbarkeit in hochdimensionalen Microarray-Daten" (Multiplicity, model validation, and reproducibility in high-dimensional microarray data, headed by the German Diabetes Center, DDZ).

The high rank of WIAS in the mathematical community was again witnessed by the fact that the long success story of transfer of knowledge via "brains" through the institute's members continued also in 2009. Five calls for professorships were received by members of WIAS, the largest number ever: Dr. Angelika Rohde accepted a junior professorship at the University of Hamburg, PD Dr. Matthias Ehrhardt a W2 professorship at the University of Wuppertal, PD Dr. Wolfgang Dreyer was awarded a

honorary professorship at the Technical University of Berlin, Dr. Gilles Blanchard received an offer for a junior professorship at the Humboldt University of Berlin, which he rejected, and then was offered a W3 professorship at the University of Potsdam. Since the institute's foundation in 1992, a total of 41 calls has been received by WIAS members, a truly remarkable output of which we are proud. The absolute highlight of 2009 was, however, the fact that Dr. Pavel Krejčí was appointed as the new director of the Institute of Mathematics of the Czech Academy of Sciences in Prague.

Six 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, WIAS members (co-)organized numerous scientific meetings throughout the world.

In addition to these "global" activities, on the "local" scale WIAS has intensified its well-established cooperation with the other mathematical institutions in Berlin, with the main attention directed toward the three Berlin universities. A big step forward was the fact that two further special chairs funded by WIAS, one at the Technical University and one at the Free University, were filled by the new heads of the Research Groups *Numerical Mathematics and Scientific Computing* and *Interacting Random Systems*, Prof. Dr. Volker John and Prof. Dr. Wolfgang König. Altogether, six leading members of WIAS, including the director and his deputy, now hold WIAS-funded special chairs at the Berlin universities.

The highlight of cooperation with the mathematical institutions in Berlin was also in 2009 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 deputy director of WIAS, Prof. Dr. Alexander Mielke, is member of MATHEON's Executive Board, PD Dr. Barbara Wagner is deputy chair of the MATHEON Council, and several members of WIAS serve as *Scientists in Charge* of the center's mathematical fields or application areas. Besides, WIAS members participated in the management of 16 of its subprojects. In turn, in 2009 up to 14 scientific collaborators and several student assistants employed at WIAS were funded by MATHEON.

Another big success story for the mathematical community of Berlin is the "Berlin Mathematical School" (BMS), which was won in the framework of the German "Exzellenzinitiative" (competition for excellence). The BMS is a graduate school for advanced mathematical studies that 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 contributed considerably to the operation of the DFG Research Training Group "Analysis, Numerics, and Optimization of Multiphase Problems" at the Humboldt University of Berlin.

Our primary aim remains unchanged: to combine fundamental research with application-oriented research, and to contribute to the advancement of innovative technologies through new scientific insights. The recent achievements give evidence that this concept, in combination with hard, continuing work on scientific details, eventually leads to success.

The main event for 2010 will be the institute's evaluation by the Senate of the Leibniz Association. All members of WIAS are looking forward to proving their excellence in this important event, just as they did with excellent results during the audit performed by the institute's Scientific Advisory Board in March 2009.

We hope that funding agencies, colleagues, and partners from industry, economy, and sciences will find this report informative and will be encouraged to cooperate with us.

Berlin, in January 2010

J. Sprekels

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1 WIAS in 2009

- 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 comprising eight scientifically independent member institutes of the *Leibniz Association*. 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 mathematical modeling to the theoretical study of the models using analytical and stochastical methods, 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. Special emphasis is devoted to the extension of the institute's traditional contacts to the scientific institutions of Eastern Europe.

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

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

1.2 Structure and Scientific Organization

1.2.1 Structure

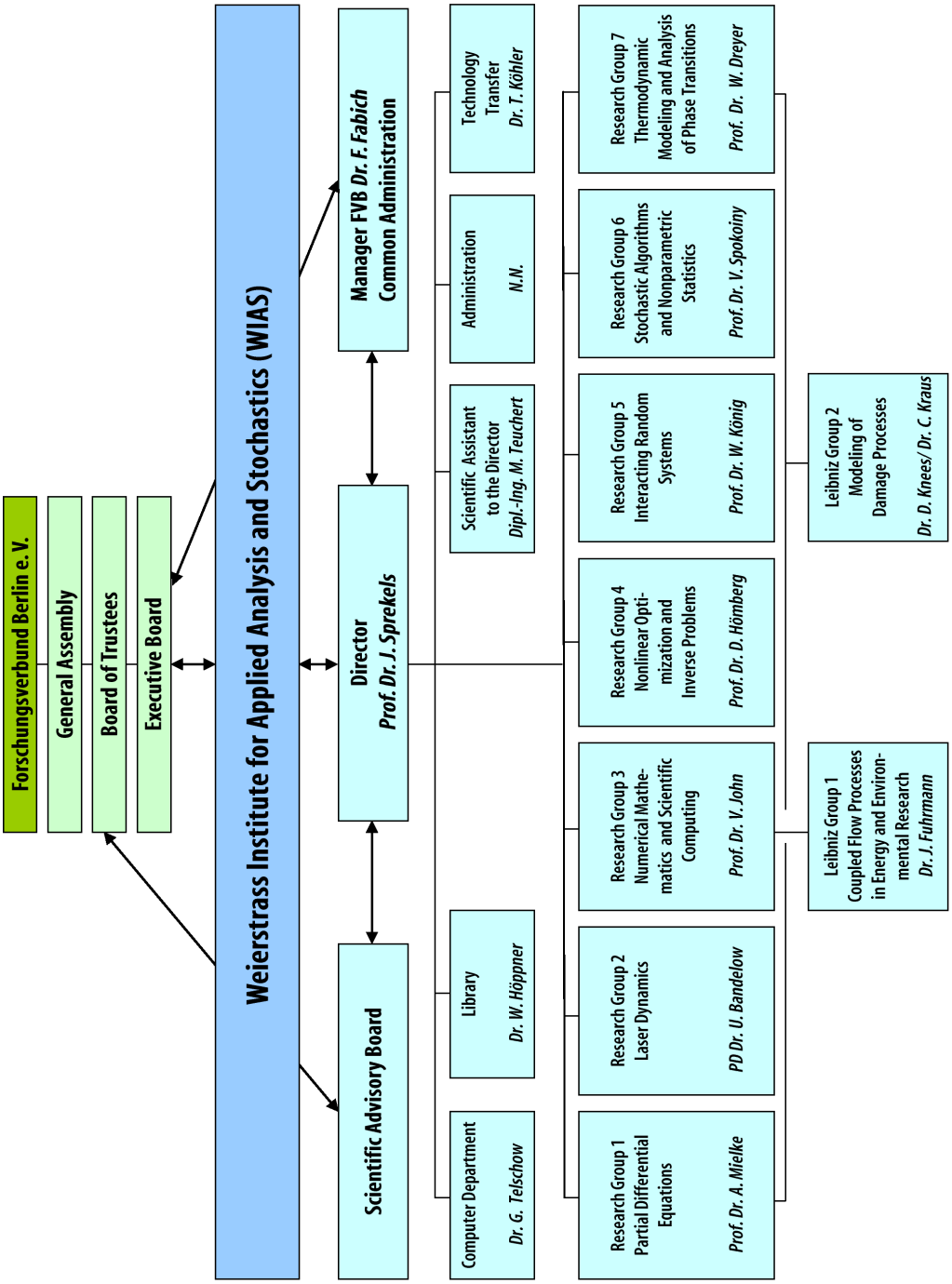
To fulfill its mission, WIAS was in 2009 organized into the departments for technical services, the seven scientific research groups, and two Leibniz groups[1]:

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" and "Leibniz group" by "LG".

LG 1. Coupled Flow Processes in Energy and Environmental Research
LG 2. Modeling of Damage Processes

The following organization chart gives an overview of the organizational structure of WIAS in 2009:



1.2.2 Main Application Areas

The research at WIAS focused in 2009 on the following *main application areas*, in which the institute has an outstanding competence in modeling, analysis, stochastic treatment, and simulation:

- **Nano- and optoelectronics**
- **Optimization and control of technological processes**
- **Phase transitions and multifunctional materials**
- **Flow and transport processes in continua**
- **Random phenomena in nature and economy**

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

- **Optical technologies** (in particular, diffractive and laser structures, semiconductor devices, and optical fibers)
- **Semiconductor crystal growth**

Recently, the institute took up the new topic of

- **Energy technology** (in particular, direct methanol fuell cells, lithium batteries, hydrogen storage, photovoltaics)

1.2.3 Contributions of the Research and Leibniz Groups

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

The table on the following page gives an overview of the main application areas to which the research and Leibniz groups contributed in 2009 in the interdisciplinary solution process described above.

Main application areas	RG 1	RG 2	RG 3	RG 4	RG 5	RG 6	RG 7	LG 1	LG 2
Nano- and optoelectronics	*	*	*	*	–	–	–	–	–
Optimization and control of technological processes	*	–	*	*	–	*	*	–	–
Phase transitions and multifunctional materials	*	–	*	*	*	–	*	–	*
Flow and transport processes in continua	*	–	*	–	–	–	*	*	–
Random phenomena in nature and economy	–	–	–	*	*	*	–	–	–

In the following, we list special research topics that were addressed in 2009 within the general framework of the main application areas. The research and Leibniz groups that contributed to the respective studies are indicated in brackets.

1. Nano- and optoelectronics

- Microelectronic devices (simulation of semiconductor devices; in RG 1 and RG 3)
- Phenomenological modeling of semiconductor heterostructures (in RG 1)
- Diffractive optics (simulation and optimization of diffractive devices; in RG 4)
- Quantum mechanical modeling of nanostructures and their consistent coupling to macroscopic models (in RG 1)
- Laser structures (multisection lasers, VCSELs, quantum dots; in RG 1 and RG 2)
- Fiber optics (modeling of optical fields in nonlinear dispersive optical media; in RG 1 and RG 2)

2. Optimization and control of technological processes

- Simulation and control in process engineering (in RG 3, RG 4, and RG 6)
- Virtual production planning (optimization and inverse modeling of multibody systems; in RG 4)
- Problems of optimal shape and topology design (in RG 4 and RG 7)
- Optimal control of multifield problems in cuntinuum mechanics (in RG 3, RG 4 and RG 7)

3. Phase transitions and multifunctional materials

- Modeling of nonlinear phenomena and phase transitions in multifunctional materials (in RG 1, RG 7, and LG 2)

– Hysteresis effects (shape memory alloys, lithium batteries, hydrogen storage, piezo effects; in RG 1 and RG 7)

– Thermomechanical modeling of phase transitions in steels (in RG 4 and RG 7)

– Modeling of damage and crack processes (phase field systems and sharp interface problems, multiscale transitions; in LG 2, RG 1, 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 3 and RG 7)

– Growth of semiconductor bulk single crystals (gallium arsenide, solar silicon, quantum dots; in RG 7)

4. Flow and transport processes in continua

– Treatment of Navier–Stokes equations (in RG 3, RG 7, and LG 1)

– Flow and mass exchange in porous media (in RG 3 and LG 1)

– Modeling of coupled electrochemical processes (fuel cells, lithium batteries, hydrogen storage; in RG 1, RG 3, and RG 7)

– Modeling of nanostructures of thin films on crystalline surfaces (fluid films, thin film solar cells; in RG 1 and RG 7)

5. Random phenomena in nature and economy

– 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 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 6 and RG 7)

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 2009, having raised a total of 2.7 million euros, from which 37 additional researchers (+ 2 outside WIAS; Dec. 31, 2009) have been financed. The fact that the funds raised in industrial collaborations could be increased to 0.6 million euros is of particular importance. In total in 2009, 26.7 per cent of the total budget of WIAS and 37.4 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 the cooperation with the mathematical institutions in Berlin was the joint operation of the DFG Research Center MATHEON "Mathematics for key technologies". Following a very successful evaluation by an international panel of referees in January 2006, MATHEON was granted a second funding period until 2010. Annually, DFG funds exceeding 5.5 million euros flow into Berlin for MATHEON. In 2009, WIAS dedicated considerable financial and personal resources to the Center: Its deputy director, Prof. A. Mielke (RG 1), was a member of MATHEON's Executive Board; PD B. Wagner (RG 7) Deputy Chairperson of its Council; and WIAS members participated in the management of 16 of its subprojects. In turn, in 2009 up to 14 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, in a joint effort within the framework of the German Initiative for Excellence in 2006. With funds exceeding one million euros per year for the BMS, which started operations in fall 2006, the efforts of the mathematical institutions of Berlin are strengthened for five years to attract excellent young Ph.D. students to the city. Among the principal investigators of this successful initiative was the deputy director of WIAS. Many other members of WIAS also contributed to the operations of the BMS.

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

This international graduate college, which is operated jointly with ETH Zürich and University of Zurich, Switzerland, is another big success of the activities of Berlin's mathematicians. The graduate college, whose first funding period runs from July 2006 to December 2011, is located at the Technical University of Berlin.

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

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

MICROPLAST

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

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

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

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

Halbleiter-Nanophotonik SFB 787

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

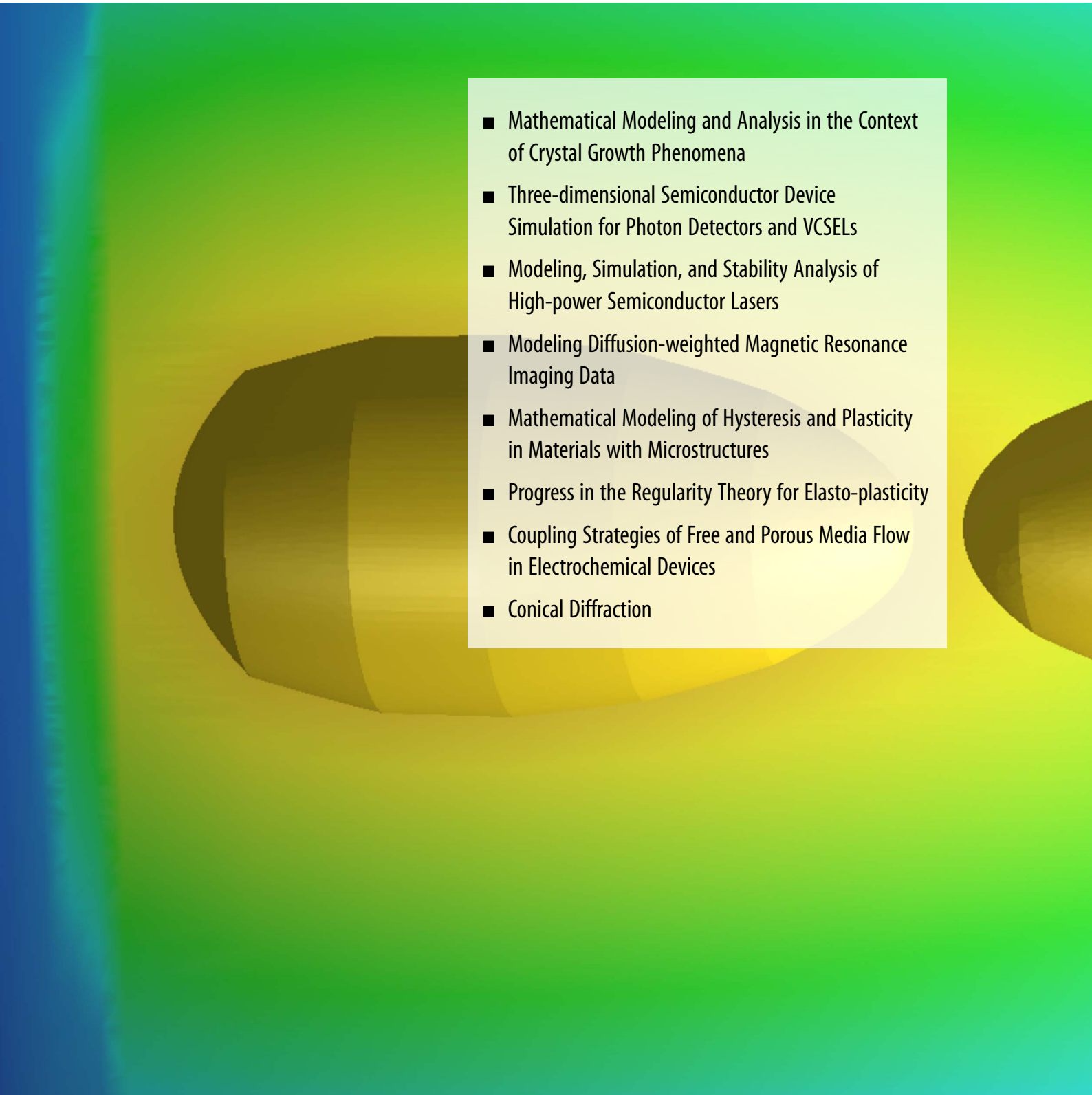
1.3.7 BMBF Project *Coupled Simulation of Particle Populations in Turbulent Flows*

This project started in July 2007. It was funded by the Federal Ministry of Education and Research within the program "Mathematics for Innovations in Industry and Services". Particle populations are studied interdisciplinarily in this project, ranging from experiments to numerical simulations (RG 3).

1.3.8 DFG Research Unit 718 *Analysis and Stochastics in Complex Physical Systems*

The second funding period of this research unit started in October 2009, when it was instituted at the Weierstrass Institute by the new head of RG 5 Prof. W. König, who is also coordinating the unit. Research is devoted to a rigorous meso- and macroscopic analysis of large interacting systems with random input on microscopic scales. One main theme is the systematic combination of tools from analysis (variational analysis, partial differential equations, etc.) and probability (large deviations, ergodic theory, etc.) to achieve goals that are out of reach of any of these disciplines alone.

2 Scientific Highlights



- Mathematical Modeling and Analysis in the Context of Crystal Growth Phenomena
- Three-dimensional Semiconductor Device Simulation for Photon Detectors and VCSELs
- Modeling, Simulation, and Stability Analysis of High-power Semiconductor Lasers
- Modeling Diffusion-weighted Magnetic Resonance Imaging Data
- Mathematical Modeling of Hysteresis and Plasticity in Materials with Microstructures
- Progress in the Regularity Theory for Elasto-plasticity
- Coupling Strategies of Free and Porous Media Flow in Electrochemical Devices
- Conical Diffraction

2.1 Mathematical Modeling and Analysis in the Context of Crystal Growth Phenomena

Wolfgang Dreyer, Olaf Klein, and Jürgen Sprekels

Introduction

The application of modern semiconductors in chips, laser devices, or solar cells involves new production processes in order to achieve higher clock rates in computers, to enhance the power of solar cells, or to reduce production costs. A deep and interdisciplinary understanding of the physical phenomena within the corresponding production chain is mandatory and can only be achieved by the use of applied mathematics and its methods *modeling*, *analysis*, and *simulation*. In particular, the artful application of mathematical methods may shorten development time, and it may even lead to patents.

This is illustrated here by means of selected aspects of two topics, namely the production of semiconductor bulk single crystals and the dissolution of unwanted precipitates in the wafer that is made from the bulk crystal. The essential mathematical context is the study of initial and boundary value problems for coupled systems of nonlinear partial differential equations involving free boundaries. Two projects within the DFG Research Center MATHEON are related to these topics, where two excellent Ph.D. studies, by P.-E. Druet (MATHEON project C9) and S.-J. Kimmerle (MATHEON project C14), have been completed.

Crystal growth in a traveling magnetic field

The most important production methods for semiconductor bulk crystals start at high temperature with a melt, and then the crystal is obtained on controlled cooling. During the so-called *Czochralski process* and its variants, the crystal is pulled from a rotating melt. Figure 1 shows a cross section of a liquid-encapsulated Czochralski (LEC) device and, on the right-hand side, a calculated temperature distribution [6].

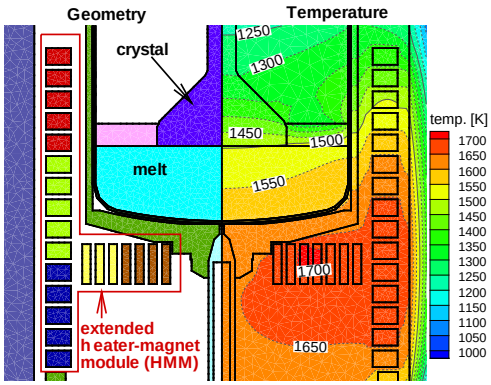
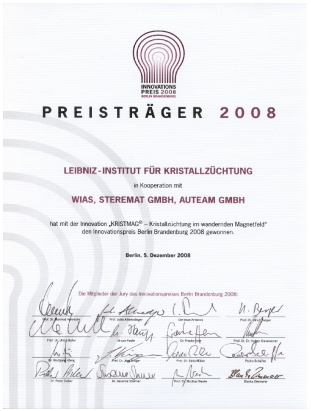


Fig. 1: *Left: LEC growth configuration with a heater-magnet module extended by two additional coils below the crucible. Right: global temperature distribution, isotherms are spaced at 50 K.*

In order to achieve a homogeneous crystal, three requirements must be met: we need, preferably, a spatially and temporally homogeneous temperature, a controlled flow within the crucible, and a convex interface between melt and crystal, requiring long-standing experience and the great art of experimentation. However, if every parameter is optimally adjusted to grow a crystal from a melt of given diameter and melt height, and if it is then decided to produce larger crystals, so that a larger crucible diameter and a larger melt height are needed, this will usually lead to a crystal of inferior quality.

This new requirement calls for tedious changes of the growth device, and new experiments to determine the new optimal parameters become necessary. One may even need some additional technical equipment to be able to produce larger crystals with the same quality. For example, traveling magnetic fields are successfully used to control the melt flow during Si growth. But the application of this new technology to the growth of III-V compounds leads to an unfavorable high power consumption, since the magnetic fields are typically generated by induction coils placed outside of the growth apparatus so that the thick walls of the pressure chamber significantly diminish the applied magnetic field; see [6].

KRISTMAG®. In this context, a consortium was founded in Berlin and Brandenburg consisting of two industrial companies (*AUTEAM Industrie-Elektronik GmbH* and *Steremat Elektrowärme GmbH*), and crystal growers, physicists, engineers, and mathematicians from WIAS, the Leibniz Institute of Crystal Growth (IKZ), Berlin, and the Institute of Electrothermic Process Engineering (ETP), Hannover, to carry out the interdisciplinary project KRISTMAG® [1]. Its aim was to investigate if an internal *heater-magnet module* (HMM), i.e., a resistance heater consisting of several coils replacing the usual heater unit within the growth apparatus, can generate traveling magnetic fields that are able to control temperature, flow, and interface boundary in the favored sense. The project, which was successfully completed in 2008, has impressively achieved these objectives: several pilot devices have been manufactured, there are some given patents and further applications for patents. The groundbreaking nature of these developments was recognized by the *Innovation Award Berlin-Brandenburg 2008*. Presently, there is a cooperation with the same partners and another company in a new project that is again funded by the "Zukunftsfonds Berlin", which deals with controlling the growth of silicon for solar cells from the melt by using traveling magnetic fields.


PREISTRÄGER 2008

LEIBNIZ-INSTITUT FÜR KRISTALLZÜCHTUNG

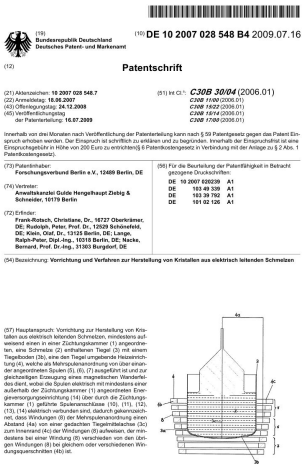
in Kooperation mit

WIAS, STEREMAT GMBH, AUTEAM GMBH

hat mit der Innovation „KRISTMAG® – Kristallzüchtung im wandernden Magnetfeld" den Innovationspreis Berlin Brandenburg 2008 gewonnen.

Berlin, 5. Dezember 2008

Fig. 2: *Innovation Award Berlin-Brandenburg 2008*


(19) Bundesrepublik Deutschland Deutsches Patent- und Markenamt

(10) DE 10 2007 028 548 B4 2009.07.16

(12) Patentschrift

(54) Bezeichnung: Vorrichtung und Verfahren zur Herstellung von Kristallen aus elektrisch leitenden Schmelzen

Fig. 3: *Patent specification*

[1] Funded by Zukunftsfonds der Stadt Berlin, by Technologiestiftung Berlin, R & D financial support from the Federal State of Brandenburg, and cofinanced by the European Union within the European Regional Development Fund (EFRE).

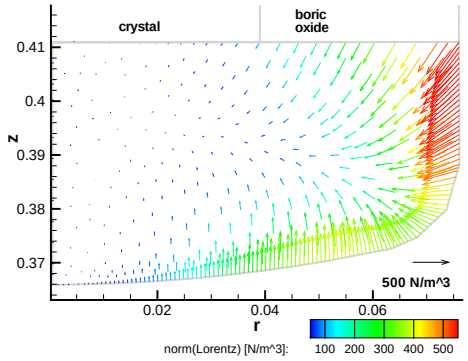
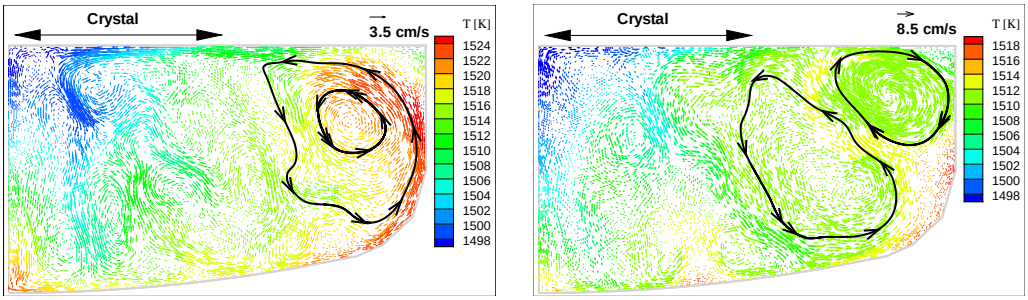


Fig. 4: *Lorentz force density in the melt. The reference vector corresponds to a force density of 50 N/m^3. The maximum of the density is around 570 N/m^3.*

On its left-hand side, Figure 5 gives a snapshot of a calculated temperature and a flow velocity distribution within the melt without the action of a Lorentz force, showing that the natural convection due to buoyancy generates an inward-rotating toroidal roll in the outer upper part of the melt.

The right-hand side of Figure 5 shows the corresponding snapshot with an acting Lorentz force as in Figure 4. In the upper outer part, the melt follows the Lorentz force in an outward-rotating toroidal roll, and a (nonpermanent) counter-rotating roll below seems to provide for a better mixing of temperature in the melt down to the middle radius.

Fig. 5: *Snapshots of velocity and temperature distribution from the simulation of the melt in the LEC configuration without Lorentz force (left-hand side) and with the Lorentz force of Figure 4. Note the different scales for temperature and velocity.*



The extended HMM arrangement in Figure 1 was motivated by means of various simulations that have proved: properly adjusted parameters and properly placed coils lead to a temporal damping of unwanted temperature oscillations and, moreover, also the shape of the crystal-melt interface may be varied. This important finding could also be observed experimentally. However, even slightest modifications of a real crystal growth installation, for example, of the system of magnetic coils, take weeks or sometimes months. During this time, neither experiments nor the production of crystals is possible. For this reason, the virtual crystal growth device, represented by a mathematical model, gives the crystal grower a competitive advantage with respect to time as well as to effort.

Mathematically, we have to solve a coupled system of partial differential equations on a complicated, nonsmooth cylindrical domain, consisting of the following equations:

1. reduced Maxwell equations

$$\frac{\partial B}{\partial t} + \operatorname{curl}\left(\frac{1}{\mu\sigma(T)}\operatorname{curl} B\right) = 0 \tag{1}$$

to compute the magnetic induction $B = (B_i)_{i=1,2,3}$,

2. the nonlinear heat conduction equation with convection due to flow velocity $v = (v_i)_{i=1,2,3}$,

$$\rho c_v \left(\frac{\partial T}{\partial t} + v \cdot \nabla T \right) = \operatorname{div}(\kappa(T)\nabla T) + \eta(T)\nabla v \cdot \cdot \nabla v + \frac{\operatorname{curl} B \cdot \operatorname{curl} B}{\mu^2 \sigma(T)}, \tag{2}$$

coupled with a nonlocal integral equation modeling heat transfer by radiation, to compute the temperature T,

3. the Boussinesq approximation of the Navier–Stokes equations to model thermally and electrically conducting viscous fluids,

$$\rho \left(\frac{\partial v}{\partial t} + v \cdot \nabla v \right) + \nabla p + \operatorname{div}\left(\eta(T)(\nabla v + (\nabla v)^{\mathrm{T}}) \right) = \rho(1 + \alpha(T - T_{\mathrm{R}}))g + \frac{1}{\mu}(\operatorname{curl} B \times B), \tag{3}$$

$$\operatorname{div} v = 0. \tag{4}$$

On the right-hand side, we have the buoyancy force, which induces unwanted eddies to a great extent, as well as the Lorentz force that controls the flow field.

This system is considered with strongly temperature-dependent physical coefficients. Moreover, one has to take free boundaries into account.

In the MATHEON project C9, P.-E. Druet achieved a mathematical breakthrough in his thesis [2] where existence and uniqueness were proved for the fully coupled system mentioned above.

For the numerical treatment of (1) and (2) without velocity in the whole growth arrangement, the software `WIAS-HiTNIHS` developed at WIAS within the MATHEON project C9 was adapted and used by O. Klein, while Ch. Lechner simulated the melt considering (2)–(4), extending and using the software NAVIER [1].

Unwanted precipitates in single-crystal gallium arsenide wafers

Thin crystalline plates, so-called *wafers*, represent the basic material to fabricate chips, lasers or photovoltaic cells. In order to homogenize the electrical, optical, and mechanical properties of a wafer, it must be subjected to a heat treatment above a certain temperature. Unfortunately, unwanted precipitates may occur during this process. In semi-insulated gallium arsenide single crystals, we find liquid droplets with an arsenic content of about 90%. In this state, the wafer cannot be used in micro- and optoelectronic applications, so that a procedure to dissolve the precipitates must be found. However, despite many experimental dissertations, the regime of precipitate evolution is undetermined up to now. For this reason, a hierarchy of verifiable models has been established at WIAS. As an example, one of these models will now be discussed in some detail.

The description of the size evolution of the precipitates is based on a thermodynamically consistent model for precipitation in gallium arsenide crystals including surface tension and bulk stresses by Dreyer and Duderstadt [3]. Within the MATHEON project C14, S.-J. Kimmerle proposed different mathematical models to describe the size evolution of liquid droplets in a crystalline solid, treating the diffusion-controlled regime of interface motion as well as the interface-controlled regime. The models take care of conservation of mass and substance and generalize the

well-known Mullins–Sekerka model for Ostwald ripening. A finite number of arsenic-rich liquid spherical droplets in a gallium arsenide crystal is considered. Droplets can shrink or grow with time, but the centers of the droplets remain fixed, while the nucleation of new droplets with time is not included in the models [5].

Due to the different scales for typical distances between droplets and typical radii of liquid droplets, one can derive from a free boundary value problem for a coupled system of diffusion equations so-called *mean-field models*. These homogenized mean-field models generalize the Lifshitz–Slyozov–Wagner model, which can be derived rigorously from the Mullins–Sekerka model.

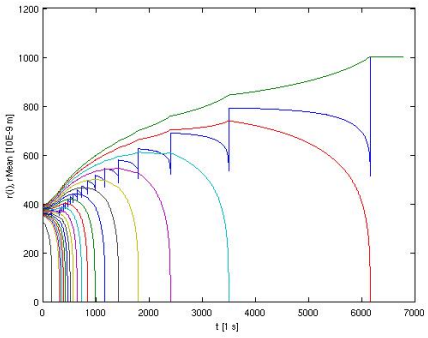
The mean-field model considers N^0 precipitates with initial radii $\{r_i(0)\}_{1\le i\le N}$ and initial mean field $\bar{u}(0)$ of the chemical potential. The evolution of the radii and the mean field is described by the system

$$\dot{r}_i = H(r_i, \bar{u}) \quad \text{and} \quad \dot{\bar{u}} = G(r_i, \bar{u})\,, \tag{5}$$

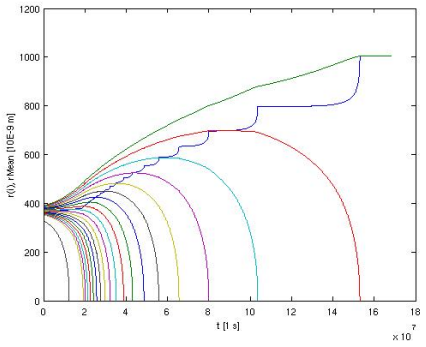
which is numerically difficult.

These mean-field models are more suitable for simulations and stability analysis than the original models. Roughly speaking, the mean-field models describe the following scenario: if we start with a fixed number of N^0 droplets, we can end up with no droplet or one droplet. Simulations show that for realistic initial data it can be expected that one droplet remains as $t \to \infty$. The simulations can be compared with times from experiments, offering a possibility to decide which model might be appropriate for the experimental situation.

$\bar{r}$ is the radius uniquely corresponding to $\bar{u}$. $\bar{r} = u_{\text{int}}^{-1}(\bar{u}) \equiv \frac{1}{\bar{u}}$.



(a) *Diffusion-controlled* regime with $D = 10^{-12}\text{m}^2$



(b) *Interface-controlled* regime with $B^I = 10^{-5}\text{mol m}^{-2}\text{s}^{-1}$

Fig. 6: *Simulations of mean-field models in diffusion- and interface-controlled regimes, showing the evolution of the mean-field radius in dark blue. In both cases, one droplet (dark green) remains, and all other droplets (other colors) dissolve. Both simulations have been done with identical initial data: 20 radii uniformly distributed between 320-400 nm, $N_0^R = 3.8 \cdot 10^{-14}$ mol, $T = 1100$ K.*

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2.2 Three-dimensional Semiconductor Device Simulation for Photon Detectors and VCSELs

Klaus Gärtner, Jens Griepentrog, and Thomas Koprucki

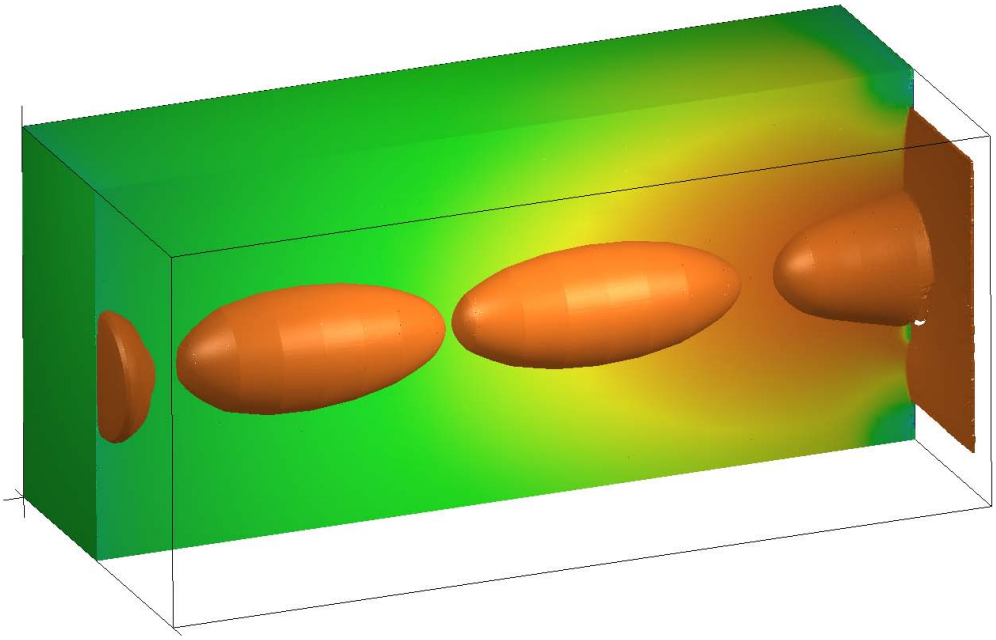

Fig. 1: *Moving electrons in an X-ray active matrix pixel sensor. The design is provided by G. Carini, National Synchrotron Light Source, Brookhaven National Lab, and contains partially depleted floating regions. Electron-hole pairs are created close to the left contact. The holes enter the contact; electrons move in the electric field to the right and get stored in a floating region. Shown are the 10-n_i isosurfaces of the electron density at 0.46, 1.54, 3.96, 8.87* ns. *90% of the 717,000 grid points are located in the right 2% of the simulation domain.*

The classical van Roosbroeck system of parabolic partial differential equations describes the transport of carriers in a semiconductor crystal lattice. Electrons and holes (missing electrons in that lattice) can recombine, interact mainly with the inner—generated by the spatial distribution of electrons and holes—and the outer electric fields and by scattering with the semiconductor lattice and the impurities, the so-called *dopant ions*. The mean free path between two scattering events is in the order of nanometers. It determines the validity of the model.

Semiconductors show an exponential dependence of currents on applied voltages, saturation effects, and multiple steady states. These properties form the basis of the semiconductor industry and make the related equations very interesting for simulations and a challenging research field for mathematics.

The large family of semiconductor devices (power switches up to megawatts, tiny sensors, computer chips, semiconductor lasers, ...) uses different basic semiconductor materials. The geometry enters via the dopant density and the contacts that inject the carriers. These characteristic lengths vary from tens of nanometers to hundreds of micrometers.

The goals of this project are:

- to develop discretization schemes that are preserving all qualitative properties of the continuous problem without additional step-size restrictions in space and time due to the scheme;
- to improve algorithms for solving the resulting nonlinear and linear equations on computers;
- to focus on selected real-world applications, to verify the methods implemented in a research code, and to answer state-of-the-art design questions in collaboration with other scientists.

Application fields

Semiconductor X-ray detectors and vertical-cavity surface-emitting lasers (VCSELs) are the application fields. Both involve light-matter interaction. Electron-hole clouds are created by photons and separate in the applied electric field of a detector. The contact currents contain the detector signal (Figure 1). In VCSELs, electrons and holes injected by different contacts are transported to the active region. Here, they recombine by emission of light. The available commercial tools do not answer the typical and highly specialized questions sufficiently.

X-ray lasers with ultra-short pulses (femtoseconds) and extreme intensity are seen as new instruments to study macromolecules. One problem is new detectors (Figure 2) able to collect the tremendous amount of data needed to turn the scattered light into valuable information on molecules and other new materials. High energy physics and X-ray astronomy face similar problems: new detectors for very different purposes with low noise, high resolution in position, time, and particle energy are designed. Often, the first amplification of the detector signal is integrated into each pixel to achieve the goal of getting both the material composition of a distant galaxy and mega-pixel resolution. VCSELs open the possibility to produce highly integrated, brilliant laser light sources with additional specific optical properties at low cost. The kinetics describing the capturing of free-moving carriers into the localized states of a nanostructured optical active region as well as the population dynamics governed by the carrier-light interaction play an important role. A comprehensive carrier transport model including these processes in detail is the aim of this project.

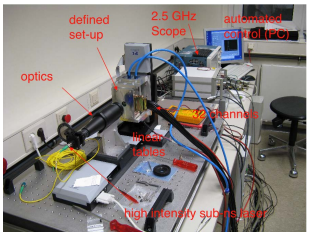

Fig. 2: *Setup to study future XFEL detector problems, Institute of Experimental Physics, University of Hamburg*

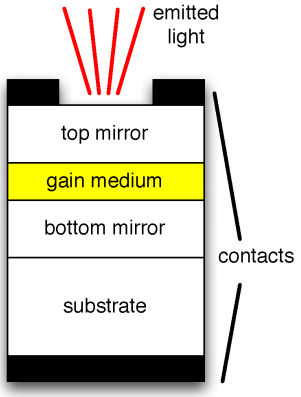

Fig. 3: *Schematic view of a VCSEL*

Mathematical and numerical aspects

Model. The electrostatic potential w, the electron density $n = n_i e^{w-\phi_n}$, and the hole density $p = n_i e^{\phi_p - w}$ are the variables of the problem. Alternative variables for n, p are the quasi-Fermi potentials ϕ_n, ϕ_p. Given a simulation domain Ω, the processes are modeled by the following coupled nonlinear system of equations: the Poisson equation for the electrostatic potential

$$-\nabla \cdot \epsilon \nabla w = C - n + p,$$

and transport equations for electrons and holes, respectively,

$$\frac{\partial n}{\partial t} - \nabla \cdot \left(n_i \mu_n e^{w} \nabla e^{-\phi_n} \right) = R, \quad \frac{\partial p}{\partial t} - \nabla \cdot \left(n_i \mu_p e^{-w} \nabla e^{\phi_p} \right) = R.$$

The doping profile, describing a fixed charge density provided by ionized atoms, is denoted by C. Further parameters are the intrinsic carrier density n_i, the dielectric permittivity ϵ, and the mobilities μ_n, μ_p. The recombination-generation rate is assumed to be of the form $R = r(x, n, p)(n_i^2 - np)$, $r \geq 0$ (Shockley–Read–Hall and Auger processes). The system is supplemented with initial and boundary conditions. Different materials with specific models of the material parameters can be assigned to subdomains Ω_i. Potentials have the natural unit "thermal voltage" ($U_T := k_B T/q_e$, k_B = Boltzmann's constant, T = temperature, q_e = charge of the electron; at room temperature $40U_T \approx 1\mathrm{V}$). Consequently, a device with an applied voltage of 1 V can show large changes in the densities and may be very far from thermodynamic equilibrium, corresponding to all applied voltages zero.

Results from analysis. With reasonable assumptions on the model data, fundamental existence results for the van Roosbroeck system on bounded Lipschitz domains Ω are available. These include existence of bounded steady states, a unique steady state for sufficiently small applied voltages, existence of unique time-dependent solutions for finite times, and the existence of a Lyapunov functional, being the free energy. Taking into account the observed saturation of the carrier speed for large electric fields ($\mu_j(.,|\nabla\phi_j|) = \mu_j(.)/(1+|\nabla\phi_j|^\beta)^{1/\beta}$ with $\beta \to 1$) results in serious mathematical and numerical difficulties.

Discretization techniques. To compute solutions, the problem is discretized in space and time. The exponential nonlinearities and the large boundary values given by the applied voltages impose strong restrictions on discretization schemes. Many schemes discussed in the mathematical literature are stable for sufficiently small time or spatial step sizes. In the case of Mock's second-order scheme, one gets a necessary stability condition for all neighboring values of the electrostatic potential: $|w_i - w_j| < (3+\sqrt{3})U_T$. The drawback are huge numbers of grid points and node positions strongly depending on the unknown discrete solution.
The Scharfetter–Gummel scheme in combination with boundary-conforming Delaunay grids (`TetGen`)[2] is stable; hence, a natural resolution defined by the data of the problem is sufficient. The related existence proofs for the fully coupled problem have been given in [1] and result in suitable averaging schemes, too. Positive approximate densities on any spatial grid of the considered class are obtained and can be improved by refinement techniques different from those often used for linear boundary value problems.

Solution techniques. The discretization results in large nonlinear systems of equations. These are linearized and solved by Newton's method. The related linear systems of equations have huge condition numbers. A tailored combination of iterative and direct methods (PARDISO)[3] is used today for problem sizes with up to 1,000,000 grid points (Figure 1). Additionally, to achieve the necessary accuracy, in particular, for contact currents, the improved evaluation of functionals [2] is unavoidable. This is done by solving a properly defined adjoint problem. The approach results in canceling one order of all small errors, from rounding to imprecisely solved linear systems. It is the key to meet strong charge conservation requirements.
Future needs, like the simulation of multi-pixel interaction and even more complex VCSEL models, require further developments. The improvement of algorithms and approximations by using analytic properties of the equations [3] and grid generation (`TetGen`) is in the focus of research at WIAS. Challenging applications are needed to judge the success beyond the line set by "lemma and proof".

Silicon detectors

The basic aim is the qualitative and quantitative understanding of detector limitations. Typical challenges for the simulation are:

- large volumes and complex geometries,
- huge density variations and large applied voltages,
- time scales from femtoseconds to seconds and a relative error of charge conservation $\leq 10^{-7}$.

[2] http://www.tetgen.org/
[3] http://www.pardiso-project.org/

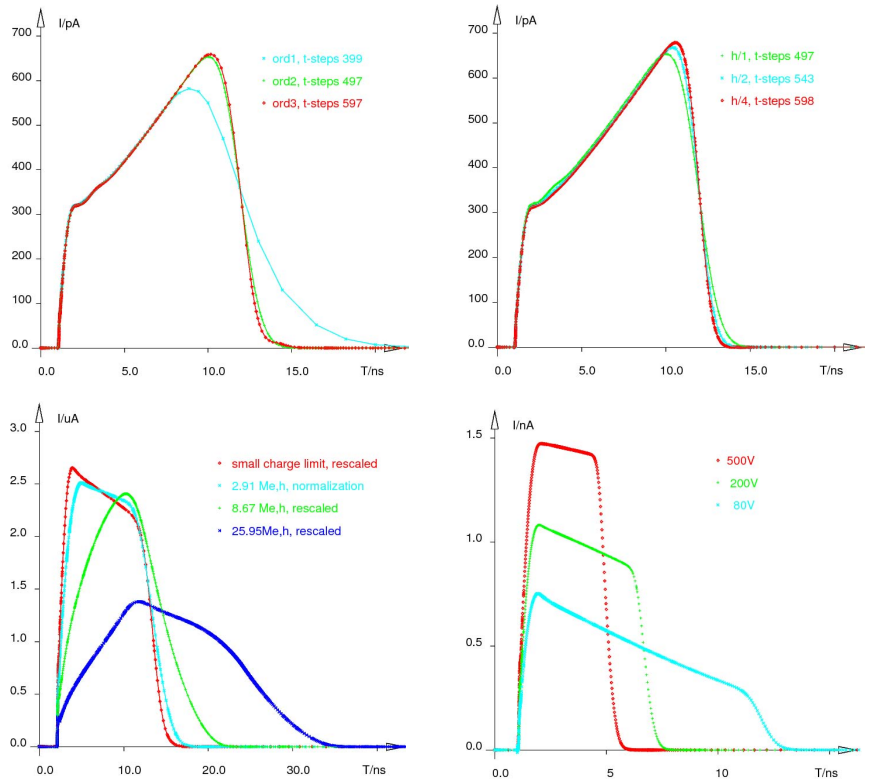

Fig. 4: *Time evolution of contact currents: influence of the time integration method for a cloud at low field (u.l.); influence of the mesh size for 80 V applied voltage (u.r.). The four time scales of the problem are: cloud creation (femto- to picoseconds), lifetime of the highly conductive plasma cloud (picoseconds to many nanoseconds), travel time of electrons and holes (nanoseconds), carrier lifetimes (milliseconds). The influence of the plasma lifetime for a cloud at high field, 200 V (l.l.); small charge limit signals at different voltages (l.r.).*

At XFEL experiments, the creation of millions of electron-hole pairs in one detector pixel is expected. This renewed the interest in the evolution of large charge clouds (Figure 4). Within the European XFEL cooperation, a measurement program is set up at the University of Hamburg to ensure design goals and to verify simulation results. Charge cloud simulations are the WIAS contribution to this program. The comparisons using literature model data agree well (Figure 5).

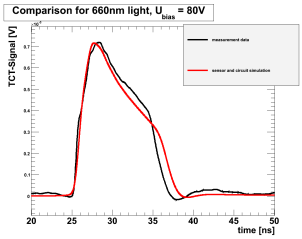

Fig. 5: *Measurement (black) versus computation based on literature data; the results suggest a field dependence of μ_n with $\beta = 1$*

VCSELs

VCSELs are semiconductor lasers emitting light in directions perpendicular to the top surface of the device. The basic VCSEL structure is a stack consisting of a gain medium sandwiched between top and bottom mirrors forming the optical cavity and contacts for the carrier injection (Figure 3). Electron-hole pairs captured in the nanostructured gain medium [4] recombine by stimulated emission of light $R_{\text{ind}} \sim g(\omega)|\Xi_0|^2 n_{\text{ph}}$ depending on the optical gain $g(\omega)$, the intensity of the lasing mode $|\Xi_0|^2$, and the number of photons n_{ph} in the lasing mode. The photon balance is determined by the emitted light and absorption in the whole device versus the generation by spontaneous and stimulated emission (R_{sp}, R_{ind}, Figure 7). Basically, we distinguish between the free-moving carriers in the bulk of the device and the carriers captured in the nanostructure. The motion of the carriers in the bulk is described by the van Roosbroeck system. The carriers confined in the nanostructure are described by rate equations. The carrier balances for each species are coupled by modeling the capture-escape processes (Figure 7).

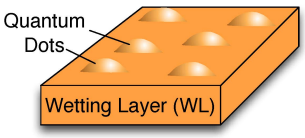

Fig. 6: *Scheme of quantum-dot (QD) wetting-layer active region. Layer thickness 5-7 nm*

For a quantum-dot wetting-layer optical active region, the rate equations describing the population

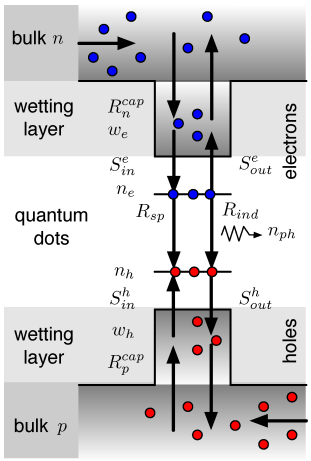

Fig. 7: *Scheme of carrier-light population dynamics for a quantum-dot active region*

dynamics of the carrier-light system (Figure 7) have the structure [5]:

$$\dot{n}_{\mathrm{ph}} = -2\kappa n_{\mathrm{ph}} + \Gamma R_{\mathrm{ind}}(n_e, n_h, n_{\mathrm{ph}}) + \beta R_{\mathrm{sp}}(n_e, n_h),$$
$$\dot{n}_b = -\frac{n_b}{\tau_b} + S_b^{\mathrm{in}} N^{\mathrm{QD}} - R_{\mathrm{ind}}(n_e, n_h, n_{\mathrm{ph}}) - R_{\mathrm{sp}}(n_e, n_h), \quad \text{for} \quad b = e, h,$$
$$\dot{w}_b = \frac{J_b(t)}{q} + \frac{n_b}{\tau_b}\frac{N^{\mathrm{WL}}}{N^{\mathrm{QD}}} - S_b^{\mathrm{in}} N^{\mathrm{WL}} - R_{\mathrm{sp}}^{\mathrm{WL}}(w_e, w_h), \quad \text{for} \quad b = e, h.$$

Here, w_e, w_h denote the carrier densities of wetting-layer states, n_e, n_h the densities of occupied quantum-dot states, and n_{ph} the number of photons in lasing mode. The scattering rates $S_e^{\mathrm{in}}, S_h^{\mathrm{in}}$ and scattering times τ_e, τ_h depend nonlinearly on the carrier densities [5].

The lasing mode is determined by the properties of the optical cavity and the nonlinear dependence of the refractive index, in particular, in the optical active region, on the wavelength and the carrier densities. This requires the coupled simulation of carrier transport, optical field, and the population dynamics of the carrier-light system. The numerical solution of this comprehensive model comprising the multilayer structure, the inherent nonlinearties, and the different length and time scales is truely challenging.

Acknowledgments

The Semiconductor Laboratory of the Max Planck Institute for Extraterrestrial Physics (HLL), Munich, has been engaged over many years in a collaboration with WIAS and opened the doors for us to the XFEL community with groups at Hamburg, Oxfordshire, and Upton, and to financial support by the European XFEL project. The extension to modern three-dimensional laser developments and new materials takes place in the project B4 *Multi-dimensional modeling and simulation of VCSEL devices* of the DFG Collaborative Research Center (SFB) 787 “Semiconductor Nanophotonics” at the Technical University of Berlin (TU). In particular, the modeling of the carrier-light interaction is done in close collaboration with the Research Group *Nonlinear Optics and Quantum Electronics* of TU Berlin. Especially, we want to thank the WIAS research groups *Partial Differential Equations* and *Laser Dynamics* for many years of close and fruitful collaboration.

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2.3 Modeling, Simulation, and Stability Analysis of High-power Semiconductor Lasers

Mark Lichtner

There is a growing interest in and demand for high-power semiconductor lasers in a variety of fields today. Traditionally, they have been used as pump sources for solid-state lasers and fiber amplifiers in telecommunications. In recent years, the technology for such lasers has been strongly driven by an increasing number of applications in display technology (laser displays, televisions, mobile beamers), medicine (surgery, photodynamic cancer therapy, fluorescence spectroscopy), free-space optical communications, and material processing (cutting, welding, marking). Semiconductor lasers are used because they have a high (up to 70%) electrical-to-optical conversion efficiency, are reliable, compact, and can be mass produced at low cost. The most important performance target for high-power laser diodes is the so-called *brightness*, which describes how well the optical power can be collimated into a narrow beam. Other performance criteria are a narrow spectral linewidth, stability in time and space, and good modulation performance.

Modeling and simulation

A simple way to increase the output power of a laser is to inject the output beam into an amplifier. Figure 1 shows a schematic top view of a *Master Oscillator Power Amplifier (MOPA)*. It consists of a single laser called the *master oscillator (MO)* combined with an amplifier on a single chip. To minimize back-reflection into the MO, the output front facet of the MOPA is anti-reflection coated. MOPAs have a good beam quality and wavelength stability, and, as has been demonstrated recently at Ferdinand Braun Institut für Höchstfrequenztechnik (FBH), can provide optical output powers of more than 10 watts. To achieve a higher output power, one simply increases the current applied to the power amplifier. A plot of the output power against the amplifier current called *power-current characteristics* is shown in Figure 2.

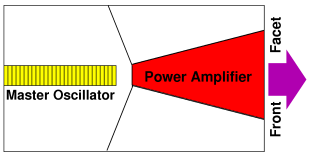

Fig. 1: *Schematic top view of a Master Oscillator Power Amplifier*

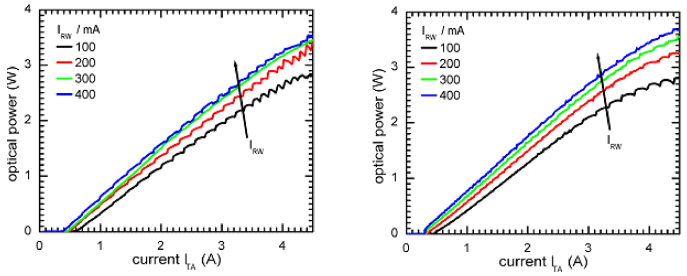

Fig. 2: *Measured (left, FBH) and simulated (right, WIAS) power-current characteristics of a MOPA [1]*

However, there are several limitations to achieve high brightness. An increase in current increases the photon density within the amplifier region. Due to the nonlinear coupling between photons and carriers, an increasing photon density reduces the carrier density. This effect is called *spatial hole burning*. It reduces the *gain* and increases the *refractive index*, so that the light starts to *self-focus*.

At high powers, this leads to *filamentation*. Filaments are “thin” concentrations of light inside the laser chip; see Figure 3.

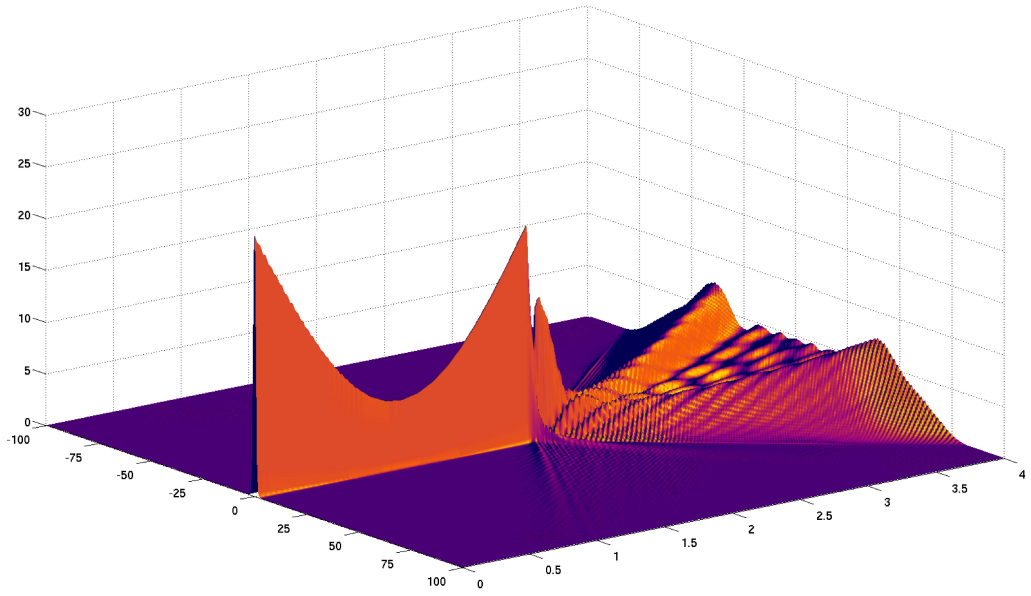

Fig. 3: *Calculated photon density distribution of a MOPA showing filamentation in the amplifier region (WIAS)*

Due to diffraction, narrow filaments cause a large divergence in the far field (the field observed at a sufficiently large distance from the laser); see Figure 4. This means that beam quality and brightness are degrading at higher output powers.

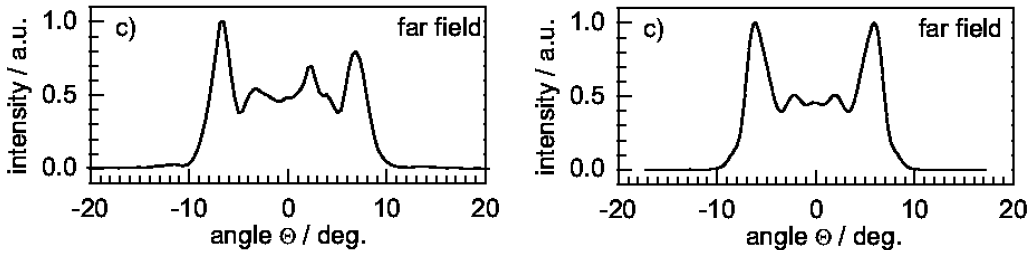

Fig. 4: *Measured (left, FBH) and simulated (right, WIAS) far field of a MOPA [1]*

Changes of the optical fields and the electronic pumping modify the temperature distributions within the device, causing effects such as thermal lensing and rollover. The effect of thermal rollover can be seen in Figure 2, where the slope of the output power declines at high amplifier currents. We showed in [1] that thermal heating effects in the amplifier cause phase changes in the residual light that is reflected back into the MO so that nearly periodic *mode jumps* occur, accompanied by dynamic instabilities; see Figure 5. Close to these mode jumps, there exist pulsations (created via Hopf bifurcations), and complicated dynamical regimes including quasiperiodic routes to chaos can be found.

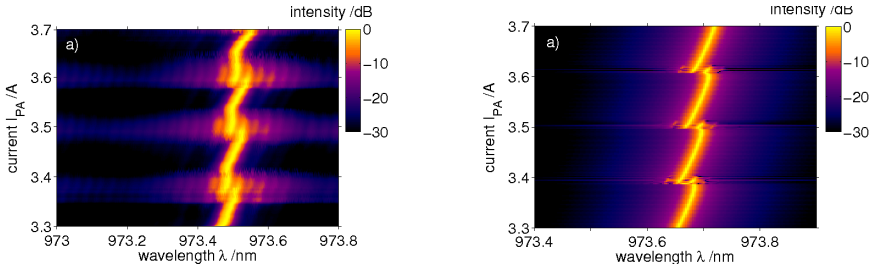

Fig. 5: *Mode jumps [1] left: experiments (FBH) right: simulations (WIAS)*

Realistic mathematical models take all the above-mentioned effects into account. Such models consist of dissipative systems of wave equations, which include field diffraction and are nonlinearly coupled to carrier [1] and heat diffusion equations. To provide an understanding of the complicated operation regimes observed in experiments, to get an understanding of the underlying physics, and to permit the exploration of novel design concepts, mathematical modeling and numerical simulation tools are essential and are becoming even more important nowadays. On the other hand, semiconductor lasers are defined by a large number of structural and geometrical design parameters. Due to the large size of high-power lasers (length of several millimeters and widths of several hundreds of micrometers) compared to the optical wavelength of $\sim$ 900 nm, the discretized equations yield about 10^7 unknown (spatial) variables, which are solved numerically for each timestep. Moreover, a fast optical field envelope dynamics on the picosecond timescale needs to be resolved with a reasonable precision compared to slow carrier relaxations, which are taking place on a nanosecond (ns) timescale. Hence, for comprehensive parameter scans of different dynamical states, time intervals of several thousands of ns need to be simulated. This is only possible by using high-performance distributed parallel computing. At WIAS, we are able to perform such investigations. Using parallel computing facilities, we were able to optimize the stability of MOPAs while maintaining a high output power of the device [5].

Well-posedness and stability analysis

The modeling needs to be accompanied by a rigorous mathematical analysis guaranteeing the well-posedness of the models [2]. This means that we have to prove the unique solvability and smooth or continuous dependence of the solutions in an appropriate *function space* setting. This theoretical knowledge supports the modeling by guaranteeing the "correctness" of the model from a pure mathematical point of view. Furthermore, this provides function space norms, which have the property that numerically calculated solutions are close to the exact solutions with respect to those norms.

Beyond basic solvability issues, rigorous mathematical descriptions for the stability and occurrence of bifurcations for different observed dynamical states need to be obtained. Moreover, the existence of finite-dimensional invariant attracting sets (*smooth invariant manifolds*) for the corresponding infinite-dimensional evolution equation model is useful for reducing the partial differential equation model to a system of ordinary differential equations [2]. Let us consider an evolution equation

$$u'(t) = f(u(t)). \tag{1}$$

Equation (1) can be considered as an abstract formulation for systems of ordinary differential equations, parabolic (heat or diffusion) equations, wave equations, or functional differential (delay differential) equations formulated in some Banach space X (using a *mild or weak formulation*). Let $u_0 \in X$ be a stationary state, i.e., $f(u_0) = 0$. Then a standard technique to determine the stability of the state u_0 for (1) is to study the stability of the linearized equation

$$u'(t) = Df(u_0)u(t). \tag{2}$$

First, one checks whether the linearized equation (2) is exponentially stable. Second, one proves that the nonlinear problem (1) is exponentially stable. For the second step, regularity questions regarding the boundedness, continuity, or smoothness of the weak solutions become important. To show the stability of (1), one performs a so-called *spectral analysis* of the linear operator $Df(u_0)$ in the Banach space X. This means that we have to solve the eigenvalue problem $Df(u_0)v = \lambda v$, where λ is a complex number, called an *eigenvalue* of the operator $Df(u_0)$, and v is an *eigenfunction*. Then a standard technique is to deduce the stability of the weak solutions to (2) from the position of all spectral points λ in the complex plane. In most cases, this can only be done numerically in a bounded region. The spectrum outside this bounded region needs to be estimated asymptotically [3]. It is a well-known standard technique, called the *"principle of linearized stability"*, to deduce the stability of the nonlinear problem (1) from the location of the spectrum λ. It is proven to be correct for ordinary differential equations and large classes of infinite-dimensional problems including parabolic and functional differential equations. However, for wave equations (used for modeling lasers) only few results are known that prove and guarantee the correctness of this procedure [3]. In fact, there exists a counterexample, which shows that this principle could fail for certain wave equations.

Different laser structures

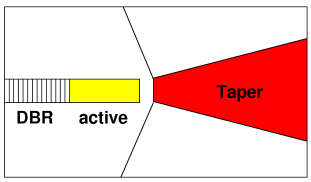

Fig. 6: *A distributed Bragg reflector tapered laser*

At WIAS, together with partners from FBH, Humboldt University of Berlin and Potsdam University, different high-power lasers were investigated. Figure 6 schematically shows a *distributed Bragg reflector (DBR) tapered laser*. DBR tapered lasers promise a better performance and stability than MOPAs. Due to an increased front facet reflectivity, the whole *cavity section* is involved in a more stable lasing process, which is additionally less sensitive to feedback effects.

Another approach to obtain high output powers with good beam quality are striped laser arrays that are stabilized by external feedback; see Figure 7. The front facet of the laser array is anti-reflection coated, and at a comparatively large (with respect to the wavelength of the light) distance of several centimeters, there is a mirror that is slightly rotated. The external mirror globally couples the stripes. By rotating the mirror, the phases of the coupling between neighboring stripes can be modified. This is used to synchronize the array to operate in a so-called stable high-power *antiphase supermode*. Using our mathematical models, we have predicted a "peculiar feature", which we call *supermode emitter doubling* of the laser array. When the angle is set to a certain specified value, which depends only on the distance of the stripes and the wavelength of the light, the number of emitters can be set to twice the number of stripes (the effective number of lasers in the array can be doubled).

Figure 8 shows the simulated photon density distribution of a broad-area laser with 40 stripes operating at a stable high-power supermode *CW* state with about 80 lasers [4]. Our theoretical prediction has recently been verified experimentally at Potsdam University.

The evolution equations for such *external cavity stabilized* lasers contain huge delay terms, which correspond to the long external cavity, being about 3×10^4 times larger than the wavelength of the light. For such large delayed systems, the number of close to *critical eigenvalues* grows to infinity for increasing delay parameter. In [6], we have given a full description of the spectrum for systems of delay differential equations with large delay.

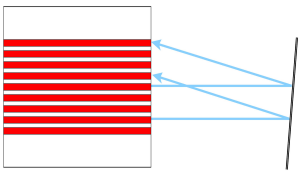

Fig. 7: *A broad-area striped laser array with angular and filtered external feedback*

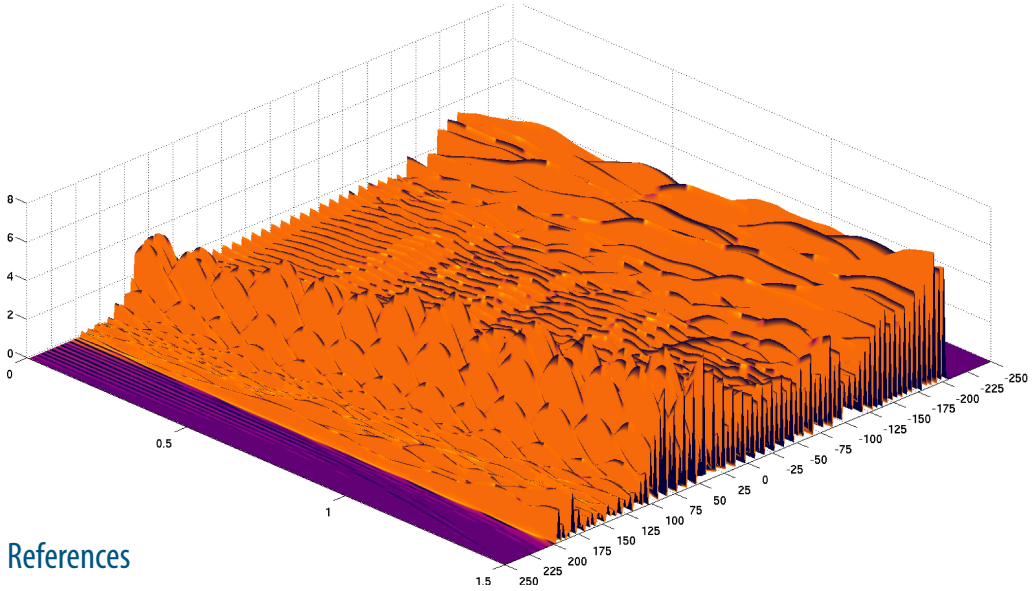

Fig. 8: *Photon densities for forward fields of a striped broad-area laser array with angular external feedback operating at a stable CW state [4] (rotated view showing the front facet)*

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2.4 Modeling Diffusion-weighted Magnetic Resonance Imaging Data

Jörg Polzehl and Karsten Tabelow

Diffusion-weighted imaging

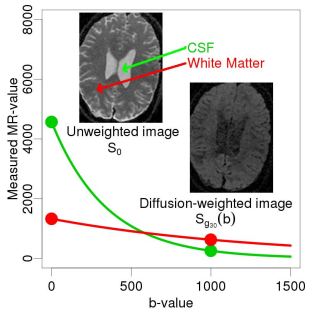

Fig. 1: *Exponential signal decay in the CSF and in WM according to* $S_{\vec{g}}(b) = S_0\, e^{-b\cdot D(\vec{g})}$

Nuclear magnetic resonance (NMR) had been known to be sensitive to the diffusion of molecules in complex systems long before the basic principles of diffusion-weighted magnetic resonance imaging (DW-MRI) were introduced in the 1980s. Since then, DW-MRI has evolved into a versatile tool for in-vivo examination of the human body that allows, in particular, to infer on the white matter anatomy of the human brain.

DW-MRI typically measures the diffusion of water, which is not isotropic in neuronal tissue, but depends on its microscopic structure. The human brain can be roughly divided into cerebrospinal fluid (CSF), gray matter (GM), and white matter (WM). The diffusion anisotropy observed in the latter is, for example, caused by restricted diffusion within its fiber bundles of nerve cell axons. The fact that DW-MRI probes microscopic structures well beyond typical image resolutions attracts broad interest in this technique. It can be used, in particular, to characterize the integrity of neuronal tissue in the central nervous system.

Different diffusion directions $\vec{g}$ can be probed by the application of corresponding bipolar magnetic field gradients with a sequence-specific parameter b (b-value). The measurement results in a three-dimensional diffusion-weighted image $S_{\vec{g}}(b)$, which is approximately exponentially attenuated relative to the unweighted image S_0 ($b = 0$). Attenuation depends on both the value b and the diffusion coefficient $D(\vec{g})$ as decay constant; see Figure 1. Typically, 15 to 100 diffusion-weighted images $S_{\vec{g}}(b)$ are measured depending on the desired angular resolutions of the directional information.

The diffusion tensor model

$$\mathcal{D} = \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{xy} & D_{yy} & D_{yz} \\ D_{xz} & D_{yz} & D_{zz} \end{pmatrix}$$

The most established model for DW-MRI is the diffusion tensor model, which is at each voxel represented by a symmetric positive definite 3×3 matrix $\mathcal{D}$. The signal attenuation law in this model reads

$$S_{\vec{g}}(b) = S_0\, e^{-b\, \vec{g}^T \mathcal{D}\, \vec{g}}. \tag{1}$$

The diffusion tensor model reduces the dimensionality of the data from up to 100 measured diffusion coefficients $D(\vec{g})$ to six diffusion tensor parameters at each voxel. It was the introduction of this diffusion tensor imaging (DTI) that made DW-MRI feasible for clinical applications, since DTI allows for an easy assessment of the local diffusion anisotropy and the main diffusion direction. The diffusion tensor can be represented by a diffusion ellipsoid where the three main axes represent

the eigenvalues of the tensor μ_i $(i = 1, 2, 3)$ in the direction of the corresponding eigenvectors. The principal eigenvector determines the main diffusion direction. Rotationally invariant quantities derived from the tensor $\mathcal{D}$ can be used to characterize intrinsic diffusion properties. One of them is the trace of the diffusion tensor

$$Tr(\mathcal{D}) = \mu_1 + \mu_2 + \mu_3 \,. \tag{2}$$

The value $\langle\mu\rangle = Tr(D)/3$ neglects the anisotropy of the diffusion and characterizes the local mean diffusivity. Another very commonly used parameter is the fractional anisotropy (FA), which is based on second-order moments of the eigenvalues and is defined as

$$FA = \sqrt{\frac{3}{2}} \sqrt{\sum_{i=1}^{3} (\mu_i - \langle\mu\rangle)^2 / \sum_{i=1}^{3} \mu_i^2} \,. \tag{3}$$

The main diffusion direction weighted by the fractional anisotropy interpreted as RGB values can be used in diagnostically helpful images; see Figure 2 for an example of such FA maps. Clinical applications detect effects of stroke and other diseases using such images or diagnostics based on the apparent diffusion coefficient (ADC) $D(\vec{g})$.

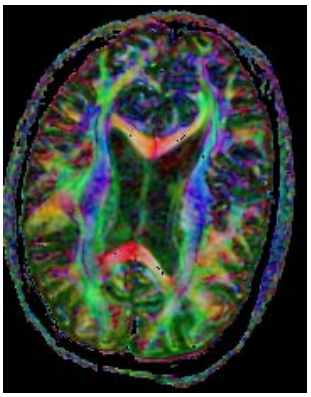

Fig. 2: *Color-coded directional map weighted with the fractional anisotropy (FA map)*

More involved applications include the identification of fiber bundles, i.e., fiber tracking, and connectivity analysis.

Adaptive smoothing of DW-MRI data

DW-MRI and hence DTI suffers from significant noise, which renders subsequent analysis or medical decisions difficult. It has been shown that noise may induce a systematically biased assessment of features like anisotropy indices. At high noise levels, in addition to the common random errors, the order of the eigenvectors of the diffusion tensor $\mathcal{D}$ is subject to a sorting bias interfering with the assessment of the main diffusion direction used for color coding in FA maps and in fiber tracking procedures. Noise reduction is therefore essential.

NMR images are acquired by fast Fourier transform from signals measured in k-space. In the case of single receiver coil systems and additive complex Gaussian noise in k-space, referred to as *thermal noise* below, this results in image grey values that follow a Rician distribution $Rice(\theta, \sigma)$. This distribution is characterized by two parameters: θ, corresponding to the signal of interest, and σ, related to the noise standard deviation in k-space. The signal attenuation of $S_{\vec{b}}$ relative to S_0 can thus be modeled by:

$$S_{\vec{g}} \sim Rice(\theta_0 \exp(-b\, D(\vec{g})),\ \sigma) \,, \quad S_0 \sim Rice(\theta_0,\ \sigma). \tag{4}$$

Additional sources of noise include effects from the cardiac cycle and respiration as well as head motion and inaccurate motion correction. The standard deviation of these noise components usually depends on the image intensity.

The current standard smoothing method, if used at all, is the application of a Gaussian kernel to the FA map, the vector field of the main diffusion direction or the diffusion tensor field. However,

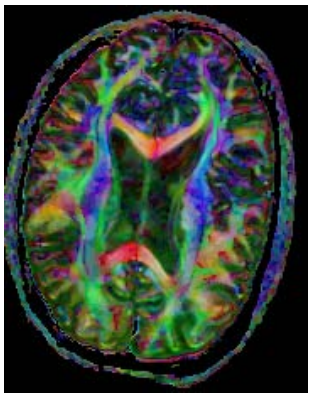

Fig. 3: *Color-coded directional map weighted with the fractional anisotropy (FA map)*

this method is known to introduce a bias at structural borders (blurring). The development of more advanced methods to overcome these limitations has been so far mainly concentrated on smoothing in tensor space. These nonlinear diffusion methods can achieve edge-preserving noise reduction but are inherently unable to reduce the estimation bias due to the presence of noise in the diffusion-weighted images $S_{\vec{g}}$.

At WIAS Berlin, we are developing new and efficient structural adaptive smoothing methods for edge-preserving image denoising. They constitute a flexible alternative to nonlinear diffusion methods for noise reduction in DTI where the structures of interest appear at multiple scales and are characterized by sharp discontinuities at tissue borders or between fiber bundles. In contrast to nonlinear diffusion methods, they provide an intrinsic stopping criterion and an automatic balance between bias and variability of parameter estimates. Furthermore, they are able to incorporate noise heteroscedasticity.

Our first attempt at the analysis of DW-MRI data in the context of the diffusion tensor model [2] employs a local homogeneity assumption on the diffusion tensor to generate adaptive weighting schemes for smoothing the diffusion-weighted images. Our algorithm is the first to take the variability of the tensor estimates into account. This approach has been refined by improving tensor estimates and variance assessment and incorporating corrections for the Rician bias [3].

Structural adaptive smoothing inspects a sequence of scales, from small to large, in an iterative procedure. Scales are defined by an exponentially increasing sequence of bandwidths h_k ($k = 0, \ldots, k^*$), with the first scale corresponding to the image resolution. At scale k, parameter estimates from the previous scale, here the estimated tensors $\hat{\mathcal{D}}_i^{(k-1)}$ and the estimated intensities $\hat{\theta}_{i,0}^{(k-1)}$, are used to infer on homogeneity and discontinuities, which is achieved by pairwise comparisons of estimates restricted to a ball of radius h_k. These comparisons take the variability of estimates into account. At each scale k and each location i, this leads to a local weighting scheme $W_i = (w_{ij}^{(k)})$ reflecting the local homogeneity structure. The weights are used to smooth the diffusion-weighted images

$$\hat{S}_{\vec{g},i}^{(k)}(b) = \sum_j w_{ij}^{(k)} \hat{S}_{\vec{g},j}(b) / \sum_j w_{ij}^{(k)} \tag{5}$$

and to infer on the parameters of the Rician distribution in voxel i and gradient direction $\vec{g}$. In a second step, new estimates $\hat{\mathcal{D}}_i^{(k)}$ of the diffusion tensor and $\hat{\theta}_{i,0}^{(k)}$ of the intensity parameters are obtained. The results of this smoothing procedure show the expected properties of noise reduction in homogeneous regions while preserving structural edges. Figure 3 provides a color-coded FA map produced from smoothed estimates for the same slice as in Figure 2.

In Figure 4, we illustrate results for an artificial data set characterized by a significant noise level. The estimated main diffusion direction and the fractional anisotropy are apparently distorted (compare the left and center figures). After structural adaptive smoothing, the noise is largely removed while the important structures (here fiber bundles) are not blurred (right figure). This property leads to a much better assessment of tensor characteristics and improved diagnostics.

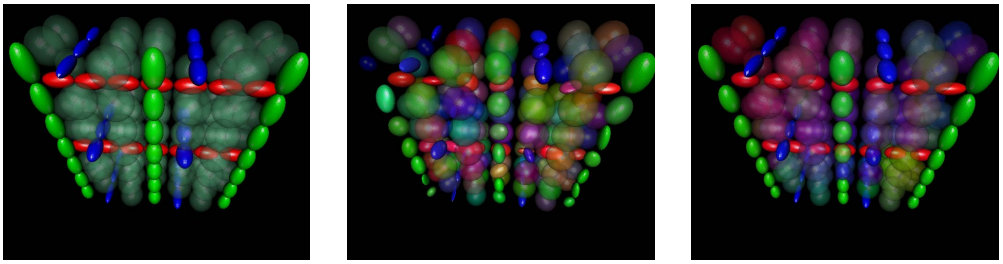

Fig. 4: *Artificial example. Left: true tensors. Center: estimates corrupted by severe noise. Right: smoothed tensor estimates.*

Structural adaptive smoothing procedures have also been successfully designed and applied for denoising and structure enhancement in imaging problems and for the analysis of functional magnetic resonance imaging experiments (fMRI), where they increase sensitivity while preserving the spatial structure of activated regions [1].

The application of these methods requires the correct assessment of noise properties and an appropriate modeling of structural properties. Structural assumptions are usually formulated in terms of local homogeneity with respect to parameters in local models. The main parameter of structural adaptive smoothing procedures can be determined by simulations for the specified model and noise distribution.

Outlook

In recent years, much progress has been made in FA-based diagnostics of brain diseases like epilepsy or stroke. With the help of structural adaptive smoothing in DTI analysis, the improved assessment of FA and the main diffusion direction is expected to refine these diagnostic tools and make new sensitive diagnostic measures possible. The correct estimation of the main diffusion direction is expected to lead to better fiber tracking results, which are the basis for connectivity maps of the human brain and, hence, for the understanding of the brain.

However, this is only a starting point. With the advances in imaging technology, there is an urgent need for further developments of structural adaptive methods. One reason is that the diffusion tensor model exploited in DTI is inherently not able to describe more complex structures like crossing fibers, which are common in the brain's white matter.

Figure 5 demonstrates the effect for the case of two fibers with an angle of 0, 60, and 90 degrees (from left to right), noiseless data generated according to (1) and 81 gradient directions. Information on crossing fibers contained in the ADC is lost in the tensor estimates, but can be modeled by approximations of the orientation density function (ODF); see [4] for the ODF approximation used.

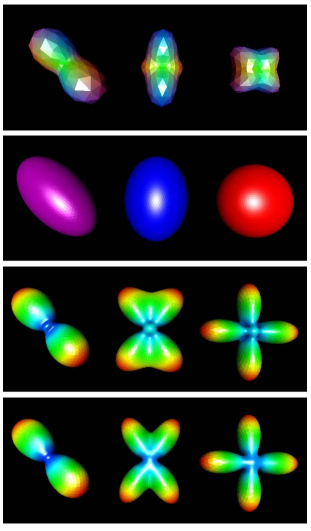

Fig. 5: *The effect of crossing fibers. Top to bottom: ADC, tensors, ODFs with spherical harmonics of order 4 and 8.*

DW-MRI data measured with high angular resolution contain the necessary information to analyze such sub-voxel structures. Thus, modeling and analysis of such data is one of the most urgent topics in current neurosciences. A series of models, e.g., spherical deconvolution, Q-ball, higher-order tensor models, and the tensor distribution function, have recently been proposed in the neuroscience literature and used to analyze DWI data. Figure 6 illustrates the normalized apparent diffusion coefficient (ADC) $\log(S_{\vec{g}}(b)) - \log(S(0))$, smoothed tensor estimates, and estimates of the orientation density function for a region with crossing fibers.

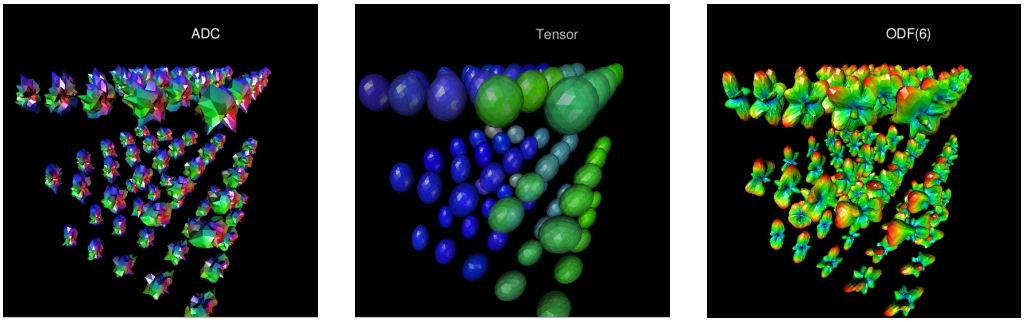

Fig. 6: *From left to right: apparent diffusion coefficient (ADC), smoothed tensor estimates, orientation density function (ODF) estimates using spherical harmonics of order 6*

All these models rely on an—in comparison to the tensor model—increased number of parameters, making them even more vulnerable to noise. Structure-preserving smoothing therefore can become an essential part of the analysis. Currently, there exists *no* practicable smoothing method. Additional aspects include, for some of these models, corrections of an intrinsic bias in the estimated fiber directions.

Software

We have developed software as a package (dti) for the R language and environment for statistical computing that is capable to perform all steps of an analysis of DW-MRI data within the diffusion tensor model from accessing medical data formats to the estimation, smoothing and visualization of the results. All illustrations within this article have been produced using this software.

Acknowledgments

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2.5 Mathematical Modeling of Hysteresis and Plasticity in Materials with Microstructures

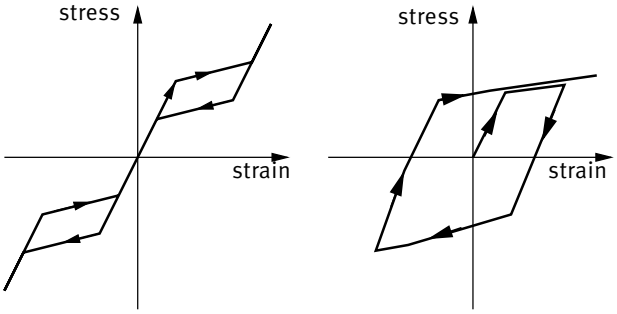
Sebastian Heinz, Alexander Mielke, and Adrien Petrov

Multifunctional and elastoplastic materials

Many modern microelectromechanical systems (MEMS) rely on specific properties of so-called *multifunctional materials*. These materials are distinguished by the fact that they combine at least two of the following properties: elastic deformability, thermal expansibility, magnetizability, polarizability switching between several stable phases. The importance is that these properties interact nontrivially in the sense that a stimulus in one property (e.g., mechanical stress, external magnetic field) generates a reaction in another property, like in a piezocrystal, where deformation generates electric current.

Shape memory alloys (SMAs) are materials that display superelasticity and have a shape memory. The latter means that a body can be deformed at room temperature in a plastic way. However, after heating up, the body returns to its original shape, which is retained after cooling. These materials became commercially available in the late 1980s. They are used in medical treatments (stents, dental braces) or microelectromechanical systems (valves, mini-grippers); cf. Figure 1.

A typical feature of multifunctional as well as elastoplastic materials is the occurrence of hysteresis, which denotes the fact that, no matter how slowly the stimulus changes, the response only follows with some delay. This is best seen under cyclic loading as is displayed in Figure 2. The enclosed area on the stress-strain diagram corresponds to the energy dissipated in the loading cycle.



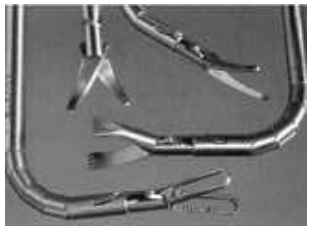
Superelastic hysteresis in SMAs Plastic hysteresis

Fig. 2: *Hysteretic cycles*

Nowadays, MEMS are primarily used as sensors, activators, grippers, values, and pumps on the sub-millimeter scale, even down to a few hundred nanometers. The miniaturization of MEMS leads to the necessity to improve the corresponding mathematical models for this material behavior.

Dental braces

Stents



Grippers

Wires

Fig. 1: *Applications using SMAs*

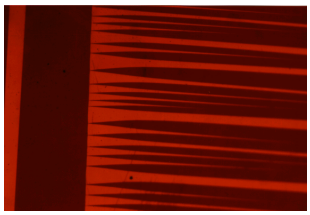


Fig. 3: *Microstructure in a CuAlNi alloy*

While the multifunctional behavior is seen on the meso- and macroscales, a microscopic investigation shows that in most cases these effects have their origin in very complicated pattern-formation processes on the microscopic scale from 10 nanometers to a few micrometers; see Figure 3. Such microstructures also occur in elastoplastic materials or in materials with damage. In the latter, the formation of microvoids or microcracks leads to a macroscopic weakening. In the former, the interaction of grains gives rise to isotropic hardening, while nanoscopic dislocation structures are needed to explain crystal plasticity.

In order to use these materials in modern devices on the different needed length scales, it is necessary to develop efficient simulation tools, which allow for testing new device concepts without needing to resort to lengthy and costly experiments or production processes. Such simulation tools are based on reliable mathematical models for the nonlinear material behavior by using suitable numerical algorithms. Hence, mathematical modeling, applied analysis, and numerics are crucial for this modern technology.

At WIAS, the following two projects, amongst others (see also the Scientific Highlights article *Progress in the Regularity Theory for Elasto-plasticity* by D. Knees on page 44), are related to this topic. The MATHEON project C18 *Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys* is devoted to the investigation and development of models for SMAs. The project *Regularizations and relaxations of time-continuous problems in plasticity* is part of the German-wide DFG Research Unit FOR 797 *Analysis and Computation of Microstructure in Finite Plasticity* and focuses on the evolution of microstructures in plastic materials.

Energetic formulation for materials with internal variables

A common feature of many multifunctional and elastoplastic materials is that they can be modeled as materials with internal variables, viz. if Ω denotes the body, then we have the displacement $u : \Omega \to \mathbb{R}^3$ and an internal variable $z : \Omega \to Z$, which incorporates all additional information needed to describe the state of the material near the material point $x \in \Omega$. For instance, z can include the magnetization, the plastic strain, or phase indicators like phase fractions. Moreover, z may describe the type of microstructure that is observed at a macroscopic point x.

The pair (u, z) thus describes the state of the material throughout the body Ω, and it is the aim to find an evolution equation for this pair, which will be a nonlinear system of partial differential equations in the time variable $t \in [0, T]$ and the space variable $x \in \Omega$. This body is modeled by an energy functional $\mathcal{E}(t, u, z)$, which is usually an integral over a stored energy density plus some term including the work of the time-dependent external forces. The derivative of $\mathcal{E}$ with respect to u provides the associated stresses, whereas the derivatives with respect to z are the associated thermomechanical driving forces. The time behavior can be described by a dissipation potential $\mathcal{R}(z, \dot{z})$ such that the derivative of $\mathcal{R}$ with respect to rate $\dot{z}$ gives the friction forces. Thus, the evolution of (u, z) is governed by the equilibrium of elastic forces and the balance of internal forces:

$$0 = \mathrm{D}_u \mathcal{E}(t, u(t), z(t)), \quad 0 \in \partial_{\dot{z}} \mathcal{R}(z(t), \dot{z}(t)) + \mathrm{D}_z \mathcal{E}(t, u(t), z(t)). \tag{BE}$$

Since hysteresis is most prominent in the case of very slow loading, it is reasonable to restrict the

modeling to the rate-independent limit where $\mathcal{R}(z,\cdot)$ is positively homogeneous of degree 1, i.e., $\mathcal{R}(z,\alpha v) = \alpha\mathcal{R}(z,v)$ for $\alpha > 0$. Since, in this case, solutions may develop jumps in time, (BE) needs to be replaced by a weaker formulation, like the so-called *energetic formulation*; see [3] for a survey. Choosing a suitable state space $\mathcal{Q}$ for (u,z) and using the dissipation distance $\mathcal{D}$ associated with $\mathcal{R}$, we say that

a pair (u,z) is called ***energetic solution*** to the rate-independent system $(\mathcal{Q},\mathcal{E},\mathcal{R})$ if

global stability: $\mathcal{E}(t,u(t),z(t)) \le \mathcal{E}(t,\bar{u},\bar{z}) + \mathcal{D}(z(t),\bar{z})$ for all comparison states $(\bar{u},\bar{z})$,

energy balance: $\mathcal{E}(t,u(t),z(t)) + \int_0^t \mathcal{R}(z,\dot{z})\,\mathrm{d}s = \mathcal{E}(0,u(0),z(0)) + \int_0^t \partial_s\mathcal{E}(s,u(s),z(s))\,\mathrm{d}s.$

The main advantage of the energetic approach is that we do not need to assume smoothness in the problem data $\mathcal{E}$ and $\mathcal{R}$ and in the solution (u,z). In particular, we do not use any linear structure in the state space $\mathcal{Q}$. This will be crucial for studying the evolution of microstructure.

Microstructures and plasticity

One way to describe microstructure in solids is the use of so-called *gradient Young measures*. The deformation gradient $\nabla u(x)$ is replaced by a probability distribution $\mu(x)$ on the set of all possible gradients in $\mathbb{R}^{3\times 3}$. This distribution is realized in materials on a representative volume element of micrometer size, while the gradient fluctuates on scales of about 10 nanometers. Typical microstructures occurring in deformation gradients are single and double laminates; see Figures 3 and 4. For a single laminate, we have

$$\mu_{\text{1-lam}}(x) = \lambda(x)\delta_{A(x)} + (1-\lambda(x))\delta_{B(x)}, \quad \text{where } A(x)-B(x) = a(x)\otimes n(x).$$

Here, $\lambda \in [0,1]$ is the volume fraction of the gradient A, and the last condition denotes the kinematic compatibility condition that guarantees that μ can be obtained as a limit of gradients. In Figure 5, we see that laminates occur in plasticity during a microindentation experiment.

As indicated in Figure 4, it is possible to build more complex microstructures by forming a laminate where each component is already a higher-order laminate. The problem is that the set Z_k of all laminates of order k does not form a convex subset of all probability measures, but rather a complicated nonlinear algebraic variety.

However, it is still possible to use the energetic formulation, where for each time t and at each point x the internal state $z(t,x)$ is a k-th order laminate. After constructing a suitable dissipation distance on Z_k and finally on $\mathcal{Q}$, it is possible to develop an evolutionary theory for laminates in elastoplastic materials or in shape memory materials; see [1, 2]. These models are the first to provide the possibility to model the spontaneous formation of true microstructure.

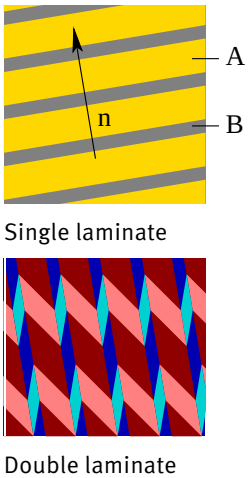


Fig. 4: *Sketch of laminates*

Fig. 5: *Laminates in plasticity*

Analysis of macroscopic models for SMAs

The energetic formulation is a versatile approach to study quite general material models including nonsmooth and hysteretic systems. In particular, it can be used to study the limit passage from

microscopic to macroscopic models. The scale bridging is one of the most important challenges in material modeling, since for many modern devices not all the relevant scales can be resolve. Thus, reliable methods are needed to derive effective models on the coarse scale. Within the energetic formulation, this can be done by a suitably adapted version of Γ-convergence. It allows us to carry out homogenization and do numerical approximation; see [6]. While these methods provide valuable qualitative information concerning the validity of limit models, they do not provide quantitative results that are necessary for practical applications. To obtain more precise information on the models at hand, one needs to specify the systems more accurately and use sharper assumptions.

So far, such quantitative convergence estimates can only be obtained for macroscopic models for SMAs where the internal variable is associated with the volume fractions of the different phases or with the effective transformation strain, like in the Souza–Auricchio model. We briefly review the mathematical model; the interested reader is referred to [5] for details. As before, the state is determined by its displacement $u : \Omega \to \mathbb{R}^3$ and the effective macroscopic transformation strain $z : \Omega \to \mathbb{R}^{3\times 3}$. Thus, the stored energy only depends on the elastic part of the strain $\mathrm{e}(u) - z$, where $\mathrm{e}(u)$ is the deformation strain $\frac{1}{2}(\nabla u + \nabla u^{\mathsf{T}})$. The stored energy potential takes the form

$$\mathcal{E}(t,u,z) = \int_\Omega \big(\tfrac{1}{2}|\mathrm{e}(u)-z|^2_{\mathbb{C}(\theta(t))} + H(\theta(t),z) + \tfrac{\nu}{2}|\nabla z|^2\big)\,\mathrm{d}x - \langle \ell(t), u\rangle,$$

where $|a|^2_{\mathbb{C}} = \sum a_{ij}C_{ijkl}a_{kl}$, and $H : \mathbb{R}^{3\times 3} \to \mathbb{R}$ is a convex hardening function, while $\ell(t)$ includes the applied mechanical loading depending on time t. Furthermore, the dissipation potential is taken in the form $\mathcal{R}(z,\dot z) = \int_\Omega \rho|\dot z(x)|\,\mathrm{d}x$, where the positive constant ρ represents an effective threshold that is needed for the initiation of the formation of martensite or for the reorientation of laminates. Moreover, following [5] it is possible to allow for temperature variations that are prescribed as a function of time.

Choosing the state space $\mathcal{Q}$ as a Hilbert space in the natural way, it can be shown that for each stable initial state (u_0, z_0) there exists at least one energetic solution. Moreover, if the function H is three times differentiable, then the solution is even unique and depends Lipschitz continuously on the initial data and the loading. From the practical point of view, it is even more important that the unique solution can be well approximated by suitable numerical procedures. If we replace the state space $\mathcal{Q}$ by a finite element subspace $\mathcal{Q}_h$ and discretize the time interval by time steps $\tau = T/N$, we can define a space-time discretized incremental minimization problem as follows:

For $k = 1, 2, \ldots, N$, find $(u_k^{\tau,h}, z_k^{\tau,h})$ in $\mathcal{Q}_h$ such that it minimizes the functional

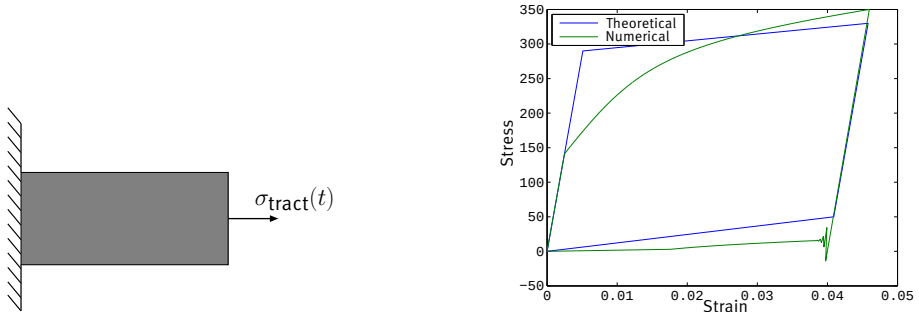
$$(u,z) \mapsto \mathcal{E}(k\tau,u,z) + \mathcal{D}(z_{k-1}^{\tau,h}, z) \text{ over } \mathcal{Q}_h.$$

One expects that the piecewise affine interpolants $(\widehat{u}^{\tau,h}, \widehat{z}^{\tau,h}) : [0,T] \to \mathcal{Q}_h$ form good approximations of the true solution. Using the Γ-convergence theory of [6] it is possible to show under quite general assumptions (no convexity of $\mathcal{E}(t,\cdot)$ needed!) that we have at least convergence of subsequences. For the Souza–Auricchio model with smooth H, one obtains a quantitative error estimate in the form

$$\|(u^{\tau,h}(t), z^{\tau,h}(t)) - (u(t), z(t))\|_{\mathcal{Q}} \le C\big(h^{\beta/2} + \tau^{1/2}\big) \text{ for all } t \in [0,T];$$

see [4]. Here, $\beta \in (0, 1]$ is determined by the higher-order regularity of the static problem only. This result seems to be the first rigorous error estimate for rate-independent evolution that does not need additional assumptions on the smoothness of the solutions to be approximated.

A short MATLAB code for the Souza–Auricchio model was implemented, starting from a plasticity code of Carstensen and Klose. It is two-dimensional and uses piecewise affine finite elements. A simulation for a uniaxial experiment in the superelastic regime is recorded in Figure 6.



(a) Setup

(b) Stress-strain diagrams for a loading cycle
green: 2D simulation; blue: 1D theory

Fig. 6: *Uniaxial tension test*

The body is fixed on the left side, submitted to the surface traction $\sigma_{\text{tract}}(t)$ on the right side, and left free on top and bottom; see Figure 6(a). Since the material parameters were chosen according to the superelastic regime, the body returns fully to the undeformed state after one loading cycle. The numerical experiments reflect this feature as it can be seen in Figure 6(b), where the output of the theoretical one-dimensional prediction of Souza–Auricchio is plotted in blue and the numerically calculated stress-strain curve is plotted in green.

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2.6 Progress in the Regularity Theory for Elasto-plasticity

Dorothee Knees

Many engineering materials on the structural scale show elastic-plastic behavior under external mechanical loadings: for small external forces the material behaves elastically, meaning that the stress in the body is uniquely determined through the strains and vice versa. In particular, after removing the external forces the body immediately returns to its initial shape. When the applied loadings pass a certain threshold, then so-called *plastic yielding* occurs due to irreversible and dissipative changes in the internal structure of the material. After removing the external loading, the new stress-free configuration of the body differs from the original one and nonzero plastic strains are present. Figure 1 shows a typical stress (σ) strain (ε) diagram of a uniaxial tension test of a metallic material under cyclic loading: 0A linear elastic response, AB plastic yielding (hardening), BC elastic unloading, CD elastic loading, DE plastic yielding.

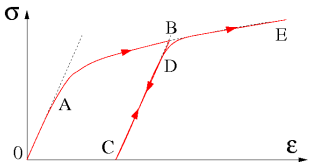

Fig. 1: *Schematic diagram of the behavior of a metallic alloy under cyclic loading*

Elastic-plastic material behavior on the macro-scale is caused by various processes on the micro-scale. The process most relevant for metals, which are materials with a polycrystalline structure, is the following: in the elastic regime, when only small forces are applied, the crystals of the material just deform according to these forces and return back to the original configuration when the forces are removed. Plastic behavior is induced by irreversible and dissipative slipping of the crystal along preferred glide planes. The slipping is mainly due to the movement of dislocations through the crystal. If the applied forces are strong enough, it is energetically favorable for the material to break and reorganize bonds between the atoms of the crystal lattice instead of deforming the crystal as a whole.

Research at WIAS in the modeling and analysis of elasto-plastic materials focuses on the following topics: in order to better understand and predict the behavior of metals, for example, during forming and manufacturing processes, it is necessary to develop models that reflect the relevant processes on the micro-scale. Models with micro-structure evolution are set up and investigated in the Research Group *Partial Differential Equations*, where also further phenomena like the shape memory effect are investigated. We refer to the Scientific Highlights article *Mathematical Modeling of Hysteresis and Plasticity in Materials with Microstructures* on page 39 for more information about the modeling issues and the related mathematical analysis. Moreover, the relation between full three-dimensional elasto-plastic models and corresponding plate and beam models involving Prandtl–Ishlinskii hysteresis operators is investigated rigorously in the Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*; see, for example, [4]. Apart from an improvement in the modeling, it is of fundamental importance to gain more insight into the analytical properties of solutions. For instance, the prediction of realistic convergence rates for numerical schemes relies on the smoothness properties of solutions of the underlying model. Furthermore, the optimal control of elastic-plastic processes, e.g., during manufacturing, requires knowledge of the regularity, as well. This is, in particular, relevant for the derivation of optimality conditions, which then may serve as a starting point for numerical simulations.

In this article, we present the newest developments concerning the smoothness or regularity properties of solutions to (classical) elasto-plastic models.

Elasto-plasticity with linear hardening

Phenomenological models describing elasto-plastic behavior rely on the assumption that the state of a material is uniquely defined through the displacements u, the stresses σ, and a finite set of so-called *internal variables*, which represent on the macroscopic level the changes in the internal structure of the material. First models were formulated by Tresca, St. Venant, Lévy, and Bauschinger in the late 19th century and were improved in the first third of the 20th century by Prandtl, Reuss, and von Mises. As a unifying general framework, B. Halphen and Nguyen Quoc Son introduced in the 70s the class of *generalized standard materials* resulting in thermodynamically admissible models for problems of this type.

As an illustration of the further discussion, we consider an elasto-plastic model with linear kinematic hardening under the assumptions that only small strains are present. It is assumed that the strain tensor ε can be decomposed additively into an elastic strain ε_e, which corresponds to the reversible part of the deformation, and a plastic strain ε_p, which represents the irreversible part. For linear kinematic hardening, the tensor ε_p is the only internal variable.

Fig. 2: *Henri Tresca (1814–1884)*

In the framework of generalized standard materials, it is postulated that there exists a stored energy functional $\mathcal{E} = \mathcal{E}(u, \varepsilon_p)$ and a convex dissipation potential $\mathcal{R} = \mathcal{R}(\varepsilon_p)$, which fully characterize the model via the relations

$$\mathrm{D}_u \mathcal{E}(t, u(t), \varepsilon_p(t)) + \ell(t) = 0, \qquad 0 \in \partial \mathcal{R}(\dot{\varepsilon}_p(t)) + \mathrm{D}_{\varepsilon_p} \mathcal{E}(t, u(t), \varepsilon_p(t)) \tag{1}$$

for t in the time interval $(0, T)$ and a time-dependent external loading ℓ. The symbols D_u and $\mathrm{D}_{\varepsilon_p}$ denote the variational derivatives of the functional $\mathcal{E}$ with respect to u and ε_p, $\partial \mathcal{R}$ is the convex subdifferential of $\mathcal{R}$ (see Figure 3), and $\dot{\varepsilon}_p$ is the time derivative of ε_p. For elasto-plasticity with linear hardening, the stored energy and the dissipation functional are defined as

$$\begin{aligned} \mathcal{E}(u, \varepsilon_p) &= \int_\Omega E(\nabla u, \varepsilon_p)\,\mathrm{d}x, \qquad \mathcal{R}(\varepsilon_p) = \int_\Omega R(\varepsilon_p)\,\mathrm{d}x, \\ E(\nabla u, \varepsilon_p) &= \tfrac{1}{2} A(\varepsilon(\nabla u) - \varepsilon_p) : (\varepsilon(\nabla u) - \varepsilon_p) + \tfrac{\gamma}{2} \left|\varepsilon_p\right|^2, \qquad R(\varepsilon_p) = \mu \left|\varepsilon_p\right|, \end{aligned} \tag{2}$$

where $\Omega \subset \mathbb{R}^d$ is the domain of the body. The first part in the energy density E accounts for the energy, which is stored in the elastic deformation $\varepsilon_e = \varepsilon(\nabla u) - \varepsilon_p$, while the second term describes the hardening behavior. The elasticity tensor A and the constants γ, μ are material-dependent quantities. According to the general framework (1), the elasto-plastic evolution model for determining the displacements $u : [0, T] \times \Omega \to \mathbb{R}^d$ and the symmetric plastic strain tensor $\varepsilon_p : [0, T] \times \Omega \to \mathbb{R}^{d \times d}_{\mathrm{sym}}$ with zero trace reads

$$0 = \ell(t, x) + \mathrm{div}_x\, A(\varepsilon(\nabla u(t, x)) - \varepsilon_p(t, x)) \quad \text{for } t \in (0, T),\ x \in \Omega, \tag{3}$$

$$0 \in \partial R(\dot{\varepsilon}_p(t, x)) + \mathrm{D}_{\varepsilon_p} E(\nabla u(t, x), \varepsilon_p(t, x)) \quad \text{for } t \in (0, T),\ x \in \Omega. \tag{4}$$

This system has to be completed with an initial condition for the internal variable and boundary conditions, like prescribed displacements or surface forces. Relation (3) represents the balance of forces relating the external loading ℓ with the internal stress $\sigma = A(\varepsilon(\nabla u) - \varepsilon_p)$. The evolution law (4) reflects the fact that the force $-\mathrm{D}_{\varepsilon_p} E$, which drives the evolution of the internal variable, first has to reach a certain threshold before the internal variable starts to evolve (see Figure 3): if

$|\mathrm{D}_{\varepsilon_p} E(u, \varepsilon_p)| < \mu$, then $\dot{\varepsilon}_p = 0$. Moreover, $\dot{\varepsilon}_p \neq 0$ if and only if $|\mathrm{D}_{\varepsilon_p} E(u, \varepsilon_p)| = \mu$.

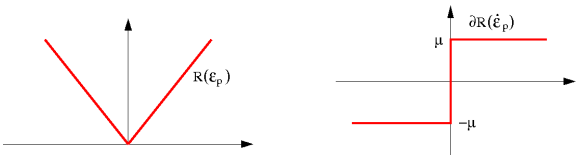

Fig. 3: *Dissipation density R and its subdifferential ∂R*

System (3)–(4) consists of a linear elliptic partial differential equation, (3), which is strongly coupled with the nonsmooth evolutionary variational inequality (4). The mathematical analysis for elasto-plastic models has its roots in the fundamental contributions by Moreau, Duvaut/Lions, and Johnson in the 1970s, where (3)–(4) was studied for $\gamma = 0$ in (2). For $\gamma > 0$, the theory of evolution equations with maximal monotone operators yields the following classical result:

Theorem. [1, 2] *Under suitable assumptions on the data, there exist a unique displacement field $u \in W^{1,1}((0,T); H_0^1(\Omega))$ and a unique plastic strain $\varepsilon_p \in W^{1,1}((0,T); L^2(\Omega))$ satisfying (3)–(4).*

The existence theorem provides $u(t) \in H_0^1(\Omega)$, meaning that the displacements are once differentiable with respect to the spatial variables. Hence, it is not clear whether the solution also satisfies the strong relation (3), which includes second spatial derivatives of u and first derivatives of ε_p. It is the topic of regularity theory to determine the actual smoothness properties of weak solutions.

The interest in regularity properties of weak solutions is also justified from the numerical point of view. A commonly used approach to solve (3)–(4) is to apply a *finite element* discretization in space and an implicit Euler discretization with respect to time. At each discrete point of time, the displacements are, e.g., approximated by continuous and piecewise affine functions, while for ε_p piecewise constant functions are used. The approximating functions are defined with respect to a computational grid of mesh size h characterizing the fineness of the approximation. In this way, problem (3)–(4) is replaced by a discrete variational inequality, which can be solved numerically. The discrete solutions converge to the solutions of the original problem provided that the fineness h of the spatial discretization and the time step size τ tend to zero. In order to construct efficient algorithms, it is of great interest to find an optimal relation between the parameters h and τ. This relies heavily on the regularity of the functions to be approximated.

Global spatial regularity

For solutions to the system (3)–(4), we proved the following global spatial regularity properties:

Theorem. [3] *Let the boundary of Ω be smooth, and assume that $\ell \in W^{1,1}(S; L^2(\Omega))$. Then, for every $\delta > 0$, we have*

$$u \in L^\infty((0,T); H^{\frac{3}{2}-\delta}(\Omega)), \quad \varepsilon_p \in L^\infty((0,T); H^{\frac{1}{2}-\delta}(\Omega)). \tag{5}$$

Theorem. [3] *If u is a scalar function and if certain compatibility conditions are satisfied between the coefficients A, γ, and the potential R, the previous result improves to*

$$u \in L^\infty((0,T); H^2(\Omega)), \quad \varepsilon_p \in L^\infty((0,T); H^1(\Omega)). \tag{6}$$

The statement (6) is in accordance with classical regularity properties for solutions of linear elliptic systems of second order on smooth domains, for which equation (3) is a particular example: if $\ell(t) \in L^2(\Omega)$ and $z(t) \in H^1(\Omega)$, then classical regularity results for linear elliptic systems imply $u(t) \in H^2(\Omega)$. This means that u is twice differentiable and has square integrable derivatives. Let us remark that local regularity properties for (3)–(4) were investigated by Seregin in [6].

The results are proved by adapting techniques for linear elliptic systems to the coupled problem and by using a reflection argument at the boundary of Ω. The proof relies on continuity properties of the data-to-solution map for the system (3)–(4). Due to the nonsmooth character of the evolution law (4), the data-to-solution map is not Lipschitz continuous from $W^{1,1}((0,T);L^2(\Omega)) \to W^{1,1}((0,T);H^1_0(\Omega)\times L^2(\Omega)) \ni (u,\varepsilon_p)$, but only with respect to some weaker norms of u and ε_p. Moreover, it is Hölder continuous with exponent $\frac{1}{2}$ from $L^\infty((0,T);L^2(\Omega)) \to L^\infty((0,T);H^1_0(\Omega)\times L^2(\Omega))$. The latter property is responsible for the exponents $\frac{3}{2}$ and $\frac{1}{2}$ in (5).

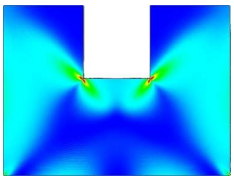

Fig. 4: *Stress distribution in an elastic material*

It is an open question for elasto-plastic models to determine which regularity properties are valid on nonsmooth domains. For linear elliptic systems, there is a rich literature, where the influence of corners and edges on the smoothness of solutions is analyzed. Figure 4 shows the stress distribution in an elastic material with high stresses at reentrant corners. Based on these results, we proved the following for solutions $u_\nu, \varepsilon_{p,\nu}$ of a regularized version of the elasto-plastic model, where R is replaced with $R_\nu(\varepsilon_p) = R(\varepsilon_p) + \frac{\nu}{2}|\varepsilon_p|^2$: assume that the elliptic operator in (3) is an isomorphism between $H^1_0(\Omega)\cap H^{1+s}(\Omega)$ and $H^{s-1}(\Omega)$ for $s \in [0,1]$. Then $u_\nu \in L^\infty((0,T); H^{1+s}(\Omega))$ and $\varepsilon_{p,\nu} \in L^\infty((0,T);H^s(\Omega))$. It is unsolved whether this remains true in the plastic limit for $\nu \to 0$.

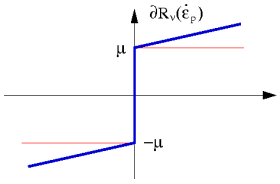

Fig. 5: *Subdifferential of the regularized potential R_ν*

A scalar example

Convergence rates for numerical schemes of elasto-plastic models are often derived assuming that the solutions along with their time derivatives have higher spatial smoothness. We discuss here an example that shows that, in spite of smooth data and geometry, higher spatial regularity in the sense of (6) is out of reach for the time derivative $\dot\varepsilon_p$. Subsequently, we present a convergence rate that relies exclusively on the smoothness properties in (5) and (6).

Spatial regularity of the time derivative. Assume that u and ε_p are scalar functions and let the energy and dissipation densities be given as

$$E(\nabla u, \varepsilon_p) = \tfrac{1}{2}\left|\nabla u - \varepsilon_p \frac{x}{|x|}\right|^2 + \tfrac{1}{2}|\varepsilon_p|^2, \qquad R(\varepsilon_p) = |\varepsilon_p|.$$

We consider a circular domain with inner radius R_1 and outer radius R_2, where the following displacement boundary conditions are imposed: $u(t,x) = 0$ if $|x| = R_1$, and $u(t,x) = t$ if $|x| = R_2$. Furthermore, $\ell \equiv 0$. The solutions depend only on $|x|$ and satisfy (6). In Figure 6, the solution ε_p and the time derivative $\dot\varepsilon_p$ are plotted. The dark blue region in the left figure indicates the elastic region ($\varepsilon_p = 0$), while in the region with lighter colors plastic yielding occurs ($\varepsilon_p \neq 0$). Due to the jump discontinuity visible in the right figure, it follows that $\dot\varepsilon_p \notin L^\infty((0,T);H^1(\Omega))$.

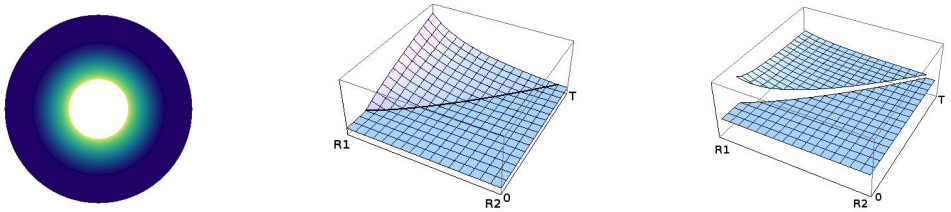

Fig. 6: *Left: Circular domain with surface plot of ε_p. Middle: ε_p versus radius and time. Right: Time derivative $\dot{\varepsilon}_p$*

Convergence rates. Based on the results (5)–(6), the following estimate is valid for the error between the continuous solution (u, ε_p) and the discrete solution $(u_h^\tau, \varepsilon_h^\tau)$ of the numerical scheme introduced in the previous section with spatial fineness h and time step size τ:

$$\sup_{0\le k\le \frac{T}{\tau}} \left\| u(k\tau) - u_h^{\tau,k} \right\|_{H^1(\Omega)} + \left\| \varepsilon_p(k\tau) - \varepsilon_{p,h}^{\tau,k} \right\|_{L^2(\Omega)} \le c(|h|^{\frac{s}{2}} + |\tau|^{\frac{1}{2}})$$

with $s = \frac{1}{2}$ in case (5) and $s = 1$ in case (6). Hence, for the example in Figure 6, the optimal relation in the discretization is $\frac{h}{\tau} = const$, which results in a predicted convergence rate of order $\frac{1}{2}$. Due to the particular structure of the example and the monotone loading, the numerical experiment even yields the higher rate 1, see Figure 7, where the error is plotted for a sequence of refinements $h_j = 2^{-j} h_0$ and $\tau_j = 2^{-j}\tau_0$ with $j \in \{1, \dots, 6\}$.

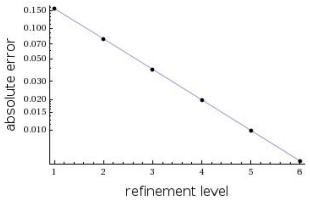

Fig. 7: *Error versus refinement level*

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2.7 Coupling Strategies of Free and Porous Media Flow in Electrochemical Devices

Matthias Ehrhardt and Jürgen Fuhrmann

The numerical simulation of coupled flows in plain and porous media is essential for many industrial and environmental problems. Here, we shortly review our work on coupling conditions between the pure liquid flow and the flow in a porous medium. We will focus on the well-studied case of parallel flow over a porous layer and investigate an electrochemical channel flow cell that includes a porous diffusion layer covering the anode. Such a structure is close to the structure of a fuel cell electrode, which usually includes a porous diffusion layer. Therefore, the investigation of the influence of the interface between free and porous media flow on solute transport processes appears to be of considerable interest [1]. We use Poiseuille-like solutions to obtain coupled free and porous media flow velocity fields, and we model the so-called *limiting current behavior* of such a cell with special emphasis on the impact of the fluid-porous interface [2].

The difficulty of finding effective coupling conditions at the interface between the channel flow and the porous layer lies in the fact that, when using stationary (Navier–)Stokes and Darcy's equations to model the flow in the two regions, the structures of the corresponding differential operators are different. Alternatively, when using the Brinkman model for the porous media, this difficulty does not occur: the continuity of velocity and stress at the interface can be satisfied. On the other hand, the validity of the Brinkman model for general porous media is discussed controversially.

We focus on three models: first, on the coupling of the free flow with a Darcy medium; secondly, the coupling with a Brinkman porous medium and, finally, we consider a three-layer configuration where the porous medium is modeled by a Brinkman transition layer overlying a Darcy porous material. From appropriate interface conditions, exact analytical solutions can be devised.

The evolution of the species concentration transported by the coupled free and porous media flow is modeled by an advection-diffusion ansatz. Also, in simple geometries, analytical solutions do not exist, and for a broad range of flow rates, asymptotic theory is not applicable even in the case without a porous layer, calling for numerical methods to obtain approximate solutions for the species concentration. The discretization method of our choice is the *finite volume method* implemented in the WIAS software `pdelib2`. Due to upwinding, it is unconditionally stable also for high flow rates and thus is able to reproduce important physical properties of the processes such as the positivity of the concentration and the local maximum principle (no overshoots).

Flow modeling

The spatial two-dimensional domain Ω under consideration consists of the free-flow domain $\Omega_f = (0, L) \times (0, H_f)$ and the porous diffusion layer $\Omega_p = (0, L) \times (-H_p, 0)$; see Figure 1.

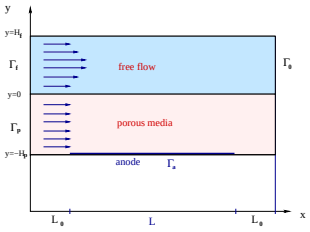

Fig. 1: *Schematic of flow cell with porous layer*

We characterize the porous medium with respect to the fluid flow by its permeability $K = K(\varepsilon)$ and, with respect to the species transport, by its dispersion coefficient D_p. The steady-state flow process in a free-flow domain is modeled by the *incompressible Navier–Stokes equations*

$$-\mu\Delta\vec{v} + (\rho\vec{v}\cdot\nabla)\vec{v} = -\nabla p, \qquad \nabla\cdot\vec{v} = 0, \qquad (x,y) \in \Omega_f. \tag{1}$$

Every flow profile in the channel satisfies the *no-slip condition* at the impermeable wall $v(y) = 0$ at $y = H_f$ and, due to the incompressibility condition $\nabla\cdot\vec{v} = 0$, one immediately obtains the continuity of the normal velocity across the fluid-porous interface at $y = 0$. We assume several flow profiles in the joint domain that are motivated by different ansatzes to model and couple the problems in the free and porous flow regions. For all flow profiles, let $\mu^{-1}\nabla p = (\delta_p, 0)^\top$ be the constant pressure gradient with $\delta_p < 0$. The different flow profiles are plotted in Figure 2.

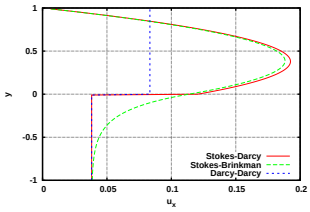

Fig. 2: *Different flow profiles*

Stokes–Darcy. We consider a Stokes flow in the channel and a Darcy flow in the porous medium

$$\mu K^{-1} v = -p_x, \qquad \nabla\cdot v = 0 \qquad \text{in } \Omega_p, \tag{2}$$

with μ being the fluid dynamic viscosity and K the permeability; see Figure 3. Generally, v denotes the volumetric average of the velocity, and p is the average of the pressure. Since the two partial differential equations (1) and (2) have different structures, the *Beavers–Joseph coupling condition* for tangential flow

$$\frac{\mathrm{d}v}{\mathrm{d}y}(0+) = \frac{\alpha}{\sqrt{K}}\left(v(0+) - v^{\mathrm{D}}\right), \quad y = 0, \tag{3}$$

was proposed in 1967, where $v^{\mathrm{D}} = -K\delta_p$ denotes the *mean filtration velocity*, and α is the *Beavers–Joseph constant* that depends on the material parameters characterizing the structure of the permeable material within the boundary region. The interface condition (3) replaces the classical condition of vanishing tangential velocity and allows for a discontinuity in the tangential velocity, taking into account rapid changes in the velocity in a small boundary layer by introducing a velocity jump. Here, the analytical solution is easily obtained [1] and is used for the transport computations.

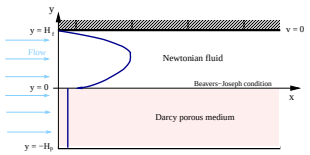

Fig. 3: *Two-layer setting for Poiseuille flow and a porous medium (Darcy): velocity is discontinuous at interface*

Stokes–Brinkman. Neale and Nader suggested in 1974 the usage of the Brinkman model:

$$-\nabla\cdot(\mu_{\mathrm{eff}}\nabla\vec{v}) + \mu K^{-1}\vec{v} = -\nabla p, \qquad \nabla\cdot\vec{v} = 0 \qquad \text{in } \Omega_p, \tag{4}$$

where $\mu_{\mathrm{eff}} = \mu/\varepsilon$ is the *effective viscosity* of the fluid in the porous media Ω_p. This model is usually used to account for *high porosity* or to impose no-slip conditions on solid walls.

This flow profile is motivated by the coupling of Stokes and Brinkman equations. This is convenient, since it involves equations of similar type, and the coupling condition of the fluid-porous interface can be described by the continuity of pressure, velocity, and stress (using μ_{eff}). For $\alpha = \sqrt{\mu_{\mathrm{eff}}/\mu}$, Neal and Nader obtained in the fluid region the same solution as Beavers and Joseph.

Stokes–Brinkman–Darcy. However, there are serious doubts about the validity of the Brinkman equation, e.g., for the case of lower porosities, whereas Darcy's law is not disputed for this case. The Brinkman model suffers from at least three limitations: first, it is only valid for materials with high porosity; secondly, the effective viscosity μ_{eff} used in this model may change discontinuously at the interface. Finally, as a rule of thumb, the Brinkman model should only be used if the Reynolds numbers $\text{Re} = \rho U L/\mu$ of the corresponding free flow is greater than 10. Here, U and L are characteristic values for the velocity and the length scale of the whole problem.

It appears to be useful to introduce a transition layer between Stokes and Darcy flow, which may be described by the Brinkman equation. For this setting, the analytical solution for the velocity profile in x-direction is given in [1]. In Figure 4, the three-layer configuration for a Poiseuille flow overlying a porous medium with Brinkman transition layer is illustrated. There is still a lower-order discontinuity in the velocity between Brinkman and Darcy layers.

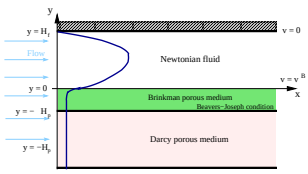

Fig. 4: *Three-layer setting for Poiseuille flow overlying a porous medium with Brinkman transition layer*

Species transport modeling

At fixed temperature T and fixed pressure p, a H_2SO_4-based electrolyte containing dissolved H_2 enters the cell at the inlet, flows over the anode, and leaves the cell at an outlet. At the inlet, the solute concentration is given by a value c_I, which depends on the pressure and the temperature. H_2 is transported to the anode and reacts at the catalytic surface according to

$$H_2 \to 2H^+ + 2e^-, \tag{5}$$

creating two electrons and two protons per reacted molecule. The amount of electrons generated during this reaction is measured as an electrical current. For high enough ion concentration due to the support electrolyte, ohmic potential drops are negligible. The reaction rate of the hydrogen oxidation (5) is large in comparison to the transport processes in the cell; therefore, we say that it is *purely transport limited*. The current I measured in such a situation is called *limiting current*.

Transport equation. According to [3, 4], the stationary species transport (convection and diffusion) in such a flow cell can be described by the partial differential equation

$$\nabla \cdot \big(D(x,y)\nabla c - c\vec{v}(x,y)\big) = 0, \qquad \nabla \cdot \vec{v} = 0 \qquad \text{in } \Omega. \tag{6}$$

Here, $c = c(x,y)$ denotes the concentration of a dissolved species, and $D = D(x,y)$ is the piecewise constant molecular diffusion coefficient. We assume for the velocity profile the form $\vec{v}(x,y) = \big(v_x(y), 0\big)^\top$ with a given x-component $v_x(y)$. In the sequel, we will shortly write $v(y)$ instead of $v_x(y)$. The values c_f, c_p denote the concentrations of the free flow and the porous inlet. The boundary concentration at the anode will be assumed to vanish, modeling a surface reaction with infinitely fast kinetics. For reaction (5), the limiting current is calculated from the amount of solute leaving the domain at the anode.

Numerical studies

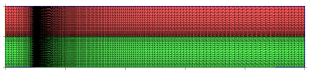

Fig. 5: Aligned computational grid

For discretizing (6), we use the Voronoi box based finite volume method on aligned grids, which has been shown to be able to reflect high flow rate asymptotics well [3]. The computational grid has been adapted in such a way that it is aligned with the flow direction: it resolves possible boundary layers (at the electrode and from both sides of the interface) and resolves the singularity at the electrode edge; for a coarse version, see Figure 5. The coupled model allows to discuss the influence of the coupling method on the possible measurement data.

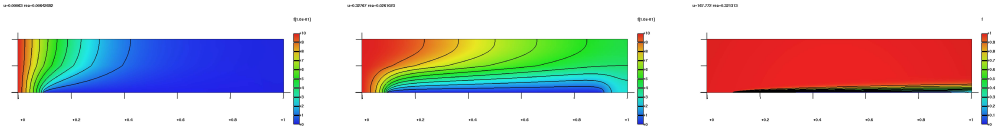

Fig. 6: Concentrations for thick layer, undivided input

Undivided input. We choose the parameters $L = 10$, $L_o = 1$, $H_p = H_f = 1$, i.e., the porous domain and the free-flow domain are of the same thickness with no divide at the inlet: $c_f = c_p = 1$. For the Stokes–Brinkman model, Figure 6 shows the concentrations for a thick porous layer and an undivided inlet for $\epsilon = 0.6$: low (left), medium (middle), and high (right) pressure gradients.

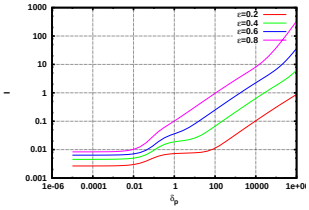

Fig. 7: Limiting current I for different porosities ε

Figure 7 essentially reveals three regimes. The low-pressure gradient regime is diffusion dominant, with a small limiting current over several magnitudes of the pressure gradient. For medium-pressure gradients, solute is transported through the cell with moderate velocity, so that a pressure gradient to the anode can build up without, however, creating a true boundary layer. At high-pressure gradients, the porous media and free flow problems essentially decouple, and the limiting current is solely determined by the porous media flow.

From Figure 8, we establish that the dependence of the limiting current on the choice between Stokes–Brinkman and Stokes–Darcy or on the choice of α, respectively, is small, within the range of typical measurement errors. However, there is a large difference to the Darcy–Darcy case.

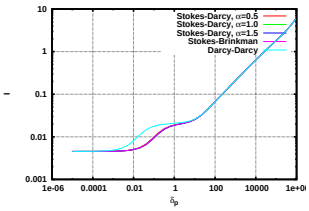

Fig. 8: Limiting current I for different models

Divided input. For divided input, i.e., $c_f = 1$, $c_p = 0$, we observe similar regimes; see Figure 9. However, it is clear that in the case of high-pressure gradients (right picture), the free flow problem and the porous media essentially decouple, which leads asymptotically to zero limiting current. Here, the limiting current is solely determined by the porous media flow. We remark that the slope is higher than that of the classical *Leveque solution*.

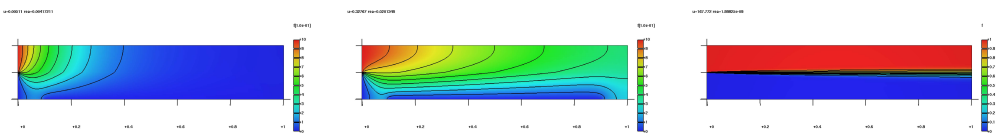

Fig. 9: Concentrations for thick layer, divided input

The weak dependence of the limiting current on the choice of α or the Stokes–Brinkman and Stokes–Darcy models can be easily recognized in Figure 8 and Figure 10; it is within the range of typical measurement errors. However, there is a large difference to the Darcy–Darcy case. On the other hand, the dependence on porous media data that are parameterized by the porosity ε is significant.

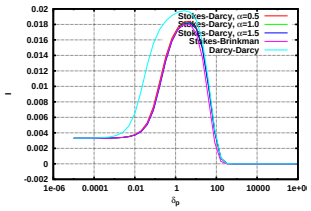

Fig. 10: *Limiting current I for different models*

Thin porous layer. Finally, we present the results of the divided input case $c_f = 1$, $c_p = 0$, for a thin porous layer. Figure 11 (left) shows again some expected behavior: for most values of pressure gradient δ_p, the limiting current increases with increasing porosity ϵ. But again, the division in the high-pressure gradient leads asymptotically to zero limiting current. Figure 11 (right) shows only a weak dependence of the limiting current on the chosen value for the slip coefficient α. But the selection of the fluid-porous model leads to strong deviations, e.g., between the Stokes–Darcy and the Stokes–Brinkman model.

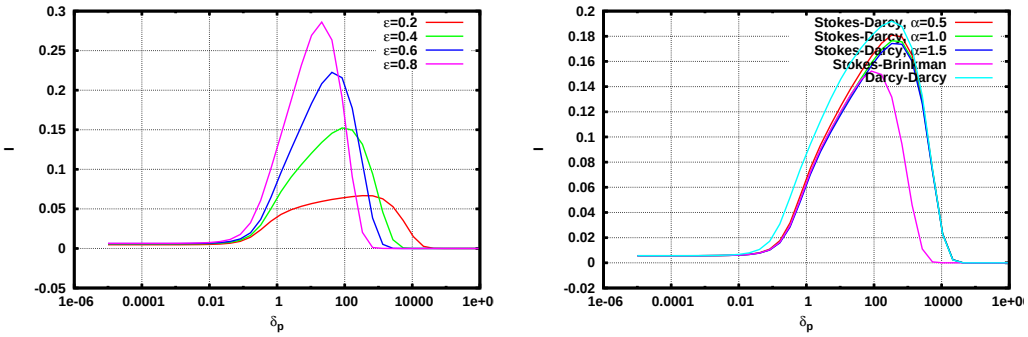

Fig. 11: *Limiting current I vs. pressure gradient δ_p*

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2.8 Conical Diffraction

Gunther Schmidt

> "It is difficult to point to another single device that has brought more important experimental information to every field of science than the diffraction grating. The physicist, the astronomer, the chemist, the biologist, the metallurgist, all use it as a routine tool of unsurpassed accuracy and precision, as a detector of atomic species to determine the characteristics of heavenly bodies and the presence of atmospheres in the planets, to study the structures of molecules and atoms, and to obtain a thousand and one items of information without which modern science would be greatly handicapped."
>
> George R. Harrison, from 1942 till 1964 Dean of Science at the Massachusetts Institute of Technology (cited from [1])

Fig. 1: *A light bulb of a flashlight seen through a transmission grating (taken from* `http://en.wikipedia.org/wiki/File:Light-bulb-grating.png`*)*

A *diffraction grating* is an optical component with a periodic pattern, which splits and diffracts light into a finite number of beams traveling in different directions. The directions of these beams depend on the direction of the input beam, on the spacing of the grating, and the wavelength of the light. Figure 1 shows a light bulb of a flashlight seen through a glass plate ruled with 830 grooves per mm parallel to the vertical axis. It depicts three main directions (so-called *transmitted orders*) for each wavelength of the input beam spectrum. The directions are governed by the *grating equation*, which for our example takes the form

$$d(\sin\theta_m + \sin\theta_i) = m\lambda\,,$$

where θ_i is the input angle of a plane wave of length λ with respect to the horizontal axis of the grating, and $d = 1.205$ μm is the grating period. If for integer m there holds the relation

$$\left| m\frac{\lambda}{d} - \sin\theta_i \right| \le 1,$$

then the solution θ_m of the grating equation is the output angle of the mth transmitted order. The order $m = 0$, which corresponds to the direct transmission of light through the grating, produces the image of the light bulb. In the other orders $m = \pm 1$, one gets a rainbow of colors corresponding to the spectrum of the illumination. Colors with increasing wavelengths (from blue to red) are diffracted at increasing angles so that the grating acts as a dispersive element.

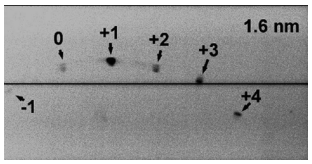

Fig. 2: *CMOS image of a conical diffraction pattern*

This is an example of so-called *classical* or *in-plane diffraction* with the incident direction lying in the plane perpendicular to the grooves. The diffracted orders also lie in the same plane. The general situation of oblique incidence of the light beam on the grating is known as *off-plane* or *conical diffraction*, because the diffracted orders lie on a cone with axis parallel to the grooves. Figure 2 depicts the conical diffraction pattern for a synchrotron radiation beam of wavelength 1.6 nm on a screen perpendicular to the grating grooves. The grating had 5,000 triangular grooves per mm, the reflected field was recorded by a complementary metal oxide semiconductor (CMOS) imager. The darkness of the spots is a measure of the *diffraction efficiencies*, which characterize how the incident field power is distributed between the different orders.

Since their invention about two centuries ago, diffraction gratings have attracted great attention,

especially for spectroscopic applications. Nowadays, modern semiconductor technologies as, for example, ion-etching techniques, paved the way for the fabrication of optical devices with complicated structural features within the length scale of optical waves. Such diffractive elements have many technological advantages and can be designed to perform functions unattainable with traditional optical devices. Recent applications cover many domains in physics and astronomy, but also applications in optical communication, information processing, together with many everyday applications, ranging from home electronics to photography equipment to security features for credit cards and banknotes.

Compared to in-plane diffraction, the conical mounting of gratings offers, due to polarization conversion, qualitatively new applications, for example, in the X-ray and extreme ultraviolet range, as perfect absorbers and local-field enhancers, color filters, artificial dielectrics, beam splitters, and wave-plate-type devices. The aim of this article is to review some results obtained at WIAS on the efficient computation of diffraction efficiencies for conical diffraction.

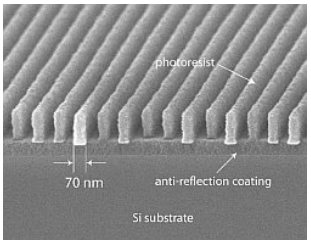

Fig. 3: *Grating etched in photoresist*

Electromagnetic theory of gratings

The directions in which a grating diffracts light are known from simple grating equations. From a grating user's point of view, it is more important to know how much of the light goes into specific directions and how this depends on the grating structure. It is now widely accepted that the prediction of efficiencies or even the design of new structures has to rely on accurate mathematical models and numerical codes for solving the full electromagnetic vector field equations.

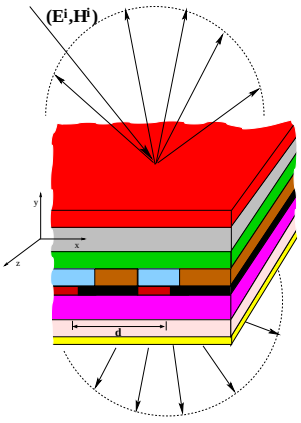

Fig. 4: *Scheme of a multilayer grating*

Maxwell formulation. Most of the grating problems are linear so that the different wavelengths diffract independently of each other. Therefore, it suffices to study the scattering of an incident electromagnetic plane wave

$$\mathbf{E}^i = \mathbf{p}\, \mathrm{e}^{i(\alpha x - \beta y + \gamma z)}\, \mathrm{e}^{-i\omega t}, \quad \mathbf{H}^i = \mathbf{q}\, \mathrm{e}^{i(\alpha x - \beta y + \gamma z)}\, \mathrm{e}^{-i\omega t}, \tag{1}$$

by the grating that is modeled as an infinite periodic structure separating two regions G_+ and G_- filled with homogeneous media. In Cartesian coordinates (x, y, z), the grating is supposed to be periodic in x-, invariant in z-direction, and located in a layer $\{|y| < H\}$. Then, illumination from G_+ implies $\beta > 0$, the frequency is $\omega = 2\pi c/\lambda$ with the speed of light c in G_+. The vector field $(\mathbf{E}, \mathbf{H})$ is a solution to the time-harmonic Maxwell equations

$$\operatorname{curl} \mathbf{E} = i\omega\mu\mathbf{H} \quad \text{and} \quad \operatorname{curl} \mathbf{H} = -i\omega\epsilon\mathbf{E}.$$

The electric permittivity ϵ and the magnetic permeability μ are given by piecewise continuous functions $\epsilon(x, y)$ and $\mu(x, y)$, which are periodic in x within the inhomogeneous grating structure. In $G_\pm$, they are constants $\epsilon_\pm, \mu_\pm$. At interfaces between different materials, where ϵ and μ are discontinuous, the tangential components of $\mathbf{E}$ and $\mathbf{H}$ have to be continuous. The components of the wave vector of the incoming field (1) satisfy $\alpha^2 + \beta^2 + \gamma^2 = \omega^2\epsilon_+\mu_+$, and they are expressed by the incidence angles

$$(\alpha, -\beta, \gamma) = \omega\sqrt{\epsilon_+\mu_+}\,(\sin\theta\cos\phi, -\cos\theta\cos\phi, \sin\phi), \quad |\theta|, |\phi| < \pi/2.$$


Lord Rayleigh

Fig. 5: *Photograph taken from* `http://www.ob-ultrasound.net/rayleigh.html`

The case $\phi = 0$ corresponds to classical diffraction, $\phi \neq 0$ characterizes conical diffraction. The periodicity of ϵ and μ together with the form of the incident wave justify that the components of $(\mathbf{E}, \mathbf{H})$ are α-quasiperiodic, i.e., they have the form $\mathrm{e}^{i\alpha x}$ times a function that is d-periodic in x. For physical reasons, the field remains bounded in y-direction. It goes back to Rayleigh [2] that, outside the grating region, the diffracted field can be represented as two series of propagating and evanescent waves, these series being known as Rayleigh expansion:

$$\begin{aligned} &(\mathbf{E}^i, \mathbf{H}^i) + \sum_{n\in\mathbb{Z}} (\mathbf{E}_n^+, \mathbf{H}_n^+)\, \mathrm{e}^{\,i(\alpha_n x + \beta_n^+ y + \gamma z)}, && y \geq H, \\ &\sum_{n\in\mathbb{Z}} (\mathbf{E}_n^-, \mathbf{B}_n^-)\, \mathrm{e}^{\,i(\alpha_n x - \beta_n^- y + \gamma z)}, && y \leq -H, \end{aligned} \tag{2}$$

with certain constant vectors $\mathbf{E}_n^\pm$, $\mathbf{H}_n^\pm$, and α_n, $\beta_n^\pm$ are given by

$$\alpha_n = \alpha + \frac{2\pi n}{d}, \quad \beta_n^\pm = \sqrt{\omega^2 \epsilon_\pm \mu_\pm - \gamma^2 - \alpha_n^2} \quad \text{with } 0 \leq \arg \beta_n^\pm < \pi\,. \tag{3}$$

Diffraction pattern. If $\beta_n^\pm \geq 0$, then the corresponding term in (2) is a plane wave (the diffracted order n), propagating with the wave vector $(\alpha_n, \pm\beta_n^\pm, \gamma)$ into $G_\pm$. This is the case only for a finite number of indices n, more precisely, the diffracted far field consists of

- reflected modes of order n if $\alpha_n^2 + \gamma^2 \leq \omega^2 \epsilon_+ \mu_+$,
- transmitted modes of order n if $\epsilon_- \mu_- > 0$ and $\alpha_n^2 + \gamma^2 \leq \omega^2 \epsilon_- \mu_-$.

The Rayleigh coefficients $(\mathbf{E}_n^\pm, \mathbf{H}_n^\pm)$ are needed to compute the energy and phase shift of the corresponding propagating modes.
For all other indices n, the imaginary part $\operatorname{Im} \beta_n^\pm > 0$; therefore, the corresponding waves decay exponentially when leaving the grating surface and are not visible in the far field. It should be noted, however, that an increasing number of applications use also the diffracted near field, so the knowledge of the Rayleigh coefficients of evanescent orders is not only of theoretical interest.

Reduction to a two-dimensional model. Due to the invariance of the geometry in z-direction, Maxwell's equations can be transformed into a two-dimensional problem. Making the ansatz

$$(\mathbf{E}, \mathbf{H})(x, y, z) = (E, H)(x, y)\, \mathrm{e}^{i\gamma z},$$

the components E_z, H_z of the vector functions $E, H : \mathbb{R}^2 \to \mathbb{C}^3$ determine the other components if $\kappa(x, y) = \sqrt{\omega^2 \epsilon(x, y) \mu(x, y) - \gamma^2} \neq 0$. Moreover, they are solutions to the Helmholtz equations

$$(\Delta + \kappa^2)\, E_z = (\Delta + \kappa^2)\, H_z = 0\,. \tag{4}$$

The continuity of the tangential components of the total fields imply the transmission conditions on the interfaces Λ between different materials

$$[E_z]_\Lambda = [H_z]_\Lambda = 0\,, \qquad \left[\frac{\gamma}{\kappa^2}\, \partial_t H_z + \frac{\omega\epsilon}{\kappa^2}\, \partial_n E_z\right]_\Lambda = \left[\frac{\gamma}{\kappa^2}\, \partial_t E_z - \frac{\omega\mu}{\kappa^2}\, \partial_n H_z\right]_\Lambda = 0\,. \tag{5}$$

Here, ∂_n and ∂_t are the normal and tangential derivatives, respectively, and $[f]_\Sigma$ denotes the jump of a function f across the interface Λ. Furthermore, (2) implies the radiation condition

$$\begin{aligned}(E_z, B_z)(x,y) &= (E_z^i, B_z^i) + \sum_{n\in\mathbb{Z}} (E_n^+, B_n^+)\, \mathrm{e}^{\,i(\alpha_n x + \beta_n^+ y)}, \qquad y \geq H,\\ (E_z, B_z)(x,y) &= \sum_{n\in\mathbb{Z}} (E_n^-, B_n^-)\, \mathrm{e}^{\,i(\alpha_n x - \beta_n^- y)}, \qquad y \leq -H.\end{aligned} \tag{6}$$

Analytical results and numerical methods

The research at WIAS on *optimization and inverse problems for diffractive structures* requires the availability of fast and reliable numerical methods for computing grating efficiencies, since apart from the trivial case of a layer system, an analytic solution of the problems is not possible. It turned out that the finite element method (FEM), which is the method of choice for complicated geometries and discontinuous coefficients, was not used in the grating community. Different groups of opticians started, with the beginning of scientific use of early computers in the late 1960s, to develop numerical methods, which are based on Rayleigh or eigenmode expansions, potential representations, or the reduction to one-dimensional differential equations. They were adopted to special geometries, and had in some cases serious convergence problems for deep grooves and high reflective materials.

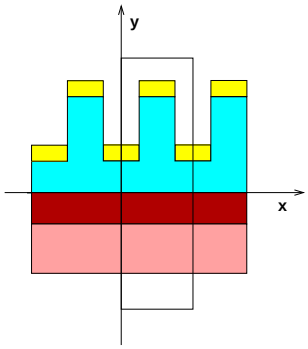

Fig. 6: *Periodic cell of a grating cross section*

Analysis. First rigorous mathematical results on existence and uniqueness of solutions of classical diffraction for gratings with arbitrary geometry and material coefficients have been obtained only after 1995. Since $\gamma = 0$, the problem (4)–(6) splits into two independent problems for E_z and H_z, called *TE* and *TM polarization*, respectively. The transmission problem for the Helmholtz equations was transformed to variational equations for quasi-periodic functions in a periodic cell with nonlocal boundary conditions imposed on the lower and upper boundary parts. It was observed that the variational forms satisfy a Gårding inequality if the nonmagnetic grating materials satisfy

$$0 \leq \arg \epsilon < \pi\,. \tag{7}$$

The formulation (4)–(6) for conical diffraction was introduced in [3]. Extending the variational approach, we could prove that the assumption (7) implies strong ellipticity of the transmission problem for the system of Helmholtz equations, which led to results similar to the TE and TM case. In particular, the equivalence to the Maxwell formulation, the existence of solutions, and their uniqueness for almost all frequencies and incident angles were shown.

FEM. The variational formulation is the basis for the finite element solution of diffraction problems; its convergence is guaranteed under condition (7). To treat also highly oscillating solutions, generalized FEMs were implemented in the WIAS program package `DiPoG`, which computes diffraction efficiencies and solves optimization problems for gratings. The optimization algorithms are based on gradient calculations, for which modified direct problems have to be solved. Let us mention that recently `DiPoG` has found important applications in the profile reconstruction of

lithography masks by using scatterometry methods. It is fair to say that the development of DiPoG and its application to various technological problems contributed to the fact that the FEM is now accepted also in the optics community.

Integral equation methods. These methods are rather popular for solving classical diffraction problems, but difficult to implement. It became apparent that integral equation methods are very efficient in certain scenarios, which combine several difficulties (nonsmooth profile curves, high wave-numbers and thin coating layers) that make them incapable of being treated by other methods. An extension of the software package IESMP, previously developed at the Karl Weierstrass Institute of Mathematics in the 80s, which is able to solve those complicated problems, is described in [4].

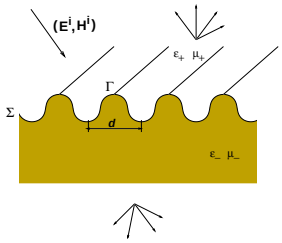

Fig. 7: *Simple grating with one surface*

Due to various requests from applications and interesting theoretical problems, the development of a similar integral equation method for conical diffraction was initiated at the end of 2007. It turned out that the two-dimensional model of conical diffraction can be transformed into singular integral equations. For example, gratings with one modulated surface lead to the equation system (cf. [5])

$$\begin{aligned}\Big((I+K_\alpha^+)V_\alpha^- + \frac{\epsilon_-\kappa_+^2}{\epsilon_+\kappa_-^2}V_\alpha^+(I-L_\alpha^-)\Big)w - \sin\phi\Big(1-\frac{\kappa_+^2}{\kappa_-^2}\Big)H_\alpha^+V_\alpha^-\tau &= -2\,E_z^i\\ \sin\phi\Big(1-\frac{\kappa_+^2}{\kappa_-^2}\Big)H_\alpha^+V_\alpha^-w + \Big((I+K_\alpha^+)V_\alpha^- + \frac{\mu_-\kappa_+^2}{\mu_+\kappa_-^2}V_\alpha^+(I-L_\alpha^-)\Big)\tau &= -2\sqrt{\frac{\mu_+}{\epsilon_+}}\,H_z^i\end{aligned} \tag{8}$$

for densities w and τ on one period Γ of the cross section of the profile curve Σ, with the integral operators ($P\in\Gamma$)

$$V_\alpha^\pm\phi(P) = 2\int_\Gamma \varphi(Q)\,\Psi_{\kappa_\pm,\alpha}(P-Q)\,d\sigma_Q\,, \qquad K_\alpha^+\phi(P) = 2\int_\Gamma \varphi(Q)\,\partial_{n(Q)}\Psi_{\kappa_+,\alpha}(P-Q)\,d\sigma_Q\,,$$
$$L_\alpha^-\phi(P) = 2\int_\Gamma \varphi(Q)\,\partial_{n(P)}\Psi_{\kappa_-,\alpha}(P-Q)\,d\sigma_Q\,, \quad H_\alpha^+\phi(P) = 2\int_\Gamma \varphi(Q)\,\partial_{t(Q)}\Psi_{\kappa_+,\alpha}(P-Q)\,d\sigma_Q\,.$$

The function $\Psi_{\kappa_\pm,\alpha}$ is the fundamental solution to the quasi-periodic Helmholtz equation

$$\Delta u + \kappa_\pm^2 u = 0$$

given for $P=(X,Y)$ by

$$\Psi_{\kappa_\pm,\alpha}(P) = \frac{i}{4}\sum_{n\in\mathbb{Z}} H_0^{(1)}\Big(\kappa_\pm\sqrt{(X-nd)^2+Y^2}\Big)\,\mathrm{e}^{ind\alpha} = \lim_{N\to\infty}\frac{i}{2d}\sum_{n=-N}^{N}\frac{\mathrm{e}^{i\alpha_n X+i\beta_n^\pm|Y|}}{\beta_n^\pm}$$

with the Hankel function of the first kind $H_0^{(1)}$. The operators $V_\alpha^\pm$ and K_α^+ are the single and double layer potentials of periodic diffraction, and H_α^+ is a principal value integral operator.

Motivated by recent proposals for the design of optical metamaterials, we allow materials with complex permeability by assuming that

$$\operatorname{Im}\epsilon_-,\ \operatorname{Im}\mu_- \geq 0 \quad \text{unless} \quad \epsilon_- \text{ and } \mu_- < 0\,. \tag{9}$$

It was shown in [5] that the integral formulation (8) is equivalent to the Maxwell formulation of conical diffraction if the single layer potential operators $V_\alpha^\pm$ have a nontrivial kernel and the integral operators

$$(\epsilon_+ + \epsilon_-)I + (\epsilon_+ - \epsilon_-)K \quad \text{and} \quad (\mu_+ + \mu_-)I + (\mu_+ - \mu_-)K \tag{10}$$

are Fredholm with index 0 in the Sobolev space $H^{1/2}(\widetilde{\Gamma})$. Here, $\widetilde{\Gamma} = \{e^{iX-Y} : (X,Y) \in \Gamma\}$ is a closed curve, and K denotes the well-known logarithmic double layer potential operator on $\widetilde{\Gamma}$. If, in addition, $\mathrm{Im}(\epsilon_- + \mu_-) > 0$, then the singular equations and, consequently, the conical diffraction problem are uniquely solvable.

Since $\widetilde{\Gamma}$ is the image of Γ under the conformal mapping e^{iz}, the smoothness properties of Γ and $\widetilde{\Gamma}$ are the same. In particular, if the profile curve Σ has no corners, then the system (8) is solvable if, besides condition (9), the relations $\epsilon_- \neq -\epsilon_+$ and $\mu_- \neq -\mu_+$ are valid. In the other case, the solvability of (8) is connected with the classical problem to determine the essential spectrum of the logarithmic double layer potential K. There exists a number $\rho > 1$ depending on the maximum angle of the profile such that the operators (10) are Fredholm with index 0 if the ratios satisfy

$$\frac{\epsilon_-}{\epsilon_+}, \frac{\mu_-}{\mu_+} \notin (-\rho, -\rho^{-1}).$$

The equation system (8) has been solved numerically using a hybrid spline-trigonometric collocation method. In various numerical tests, also for real-world problems, optimal-order convergence was confirmed.

Outlook. The development of the numerical algorithm also for gratings with multiple interfaces and its implementation will be carried out in close cooperation with L. Goray (St. Petersburg). His company I.I.G., Inc., developed the only commercially available software package *PCGrate* ® for classical diffraction, which uses integral equation methods. It is planned to extend this package to conical diffraction by including our algorithms. Another application of the integral equation approach will be the numerical computation of shape derivatives for conical diffraction, which have been derived within the Ph.D. thesis of N. Kleemann.

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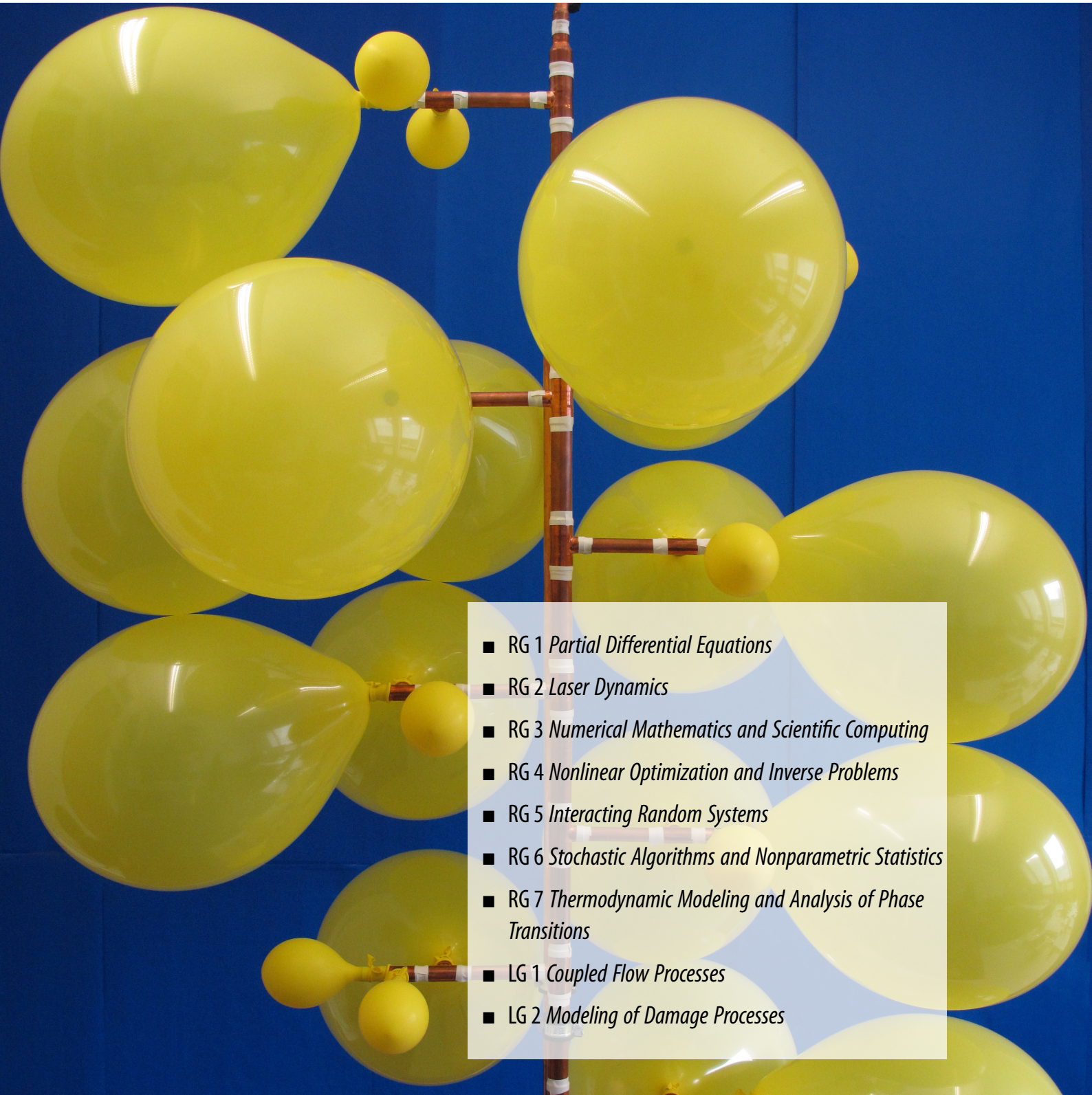
3 Groups' Essentials



- RG 1 *Partial Differential Equations*
- RG 2 *Laser Dynamics*
- RG 3 *Numerical Mathematics and Scientific Computing*
- RG 4 *Nonlinear Optimization and Inverse Problems*
- RG 5 *Interacting Random Systems*
- RG 6 *Stochastic Algorithms and Nonparametric Statistics*
- RG 7 *Thermodynamic Modeling and Analysis of Phase Transitions*
- LG 1 *Coupled Flow Processes*
- LG 2 *Modeling of Damage Processes*

3.1 Research Group 1 "Partial Differential Equations"

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

- Modeling of optoelectronic devices including quantum effects
- Multifunctional materials and plasticity

The methods involve topics from pure functional analysis, mathematical physics, pure and applied analysis, calculus of variations, and numerical analysis:

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

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

Multifunctional materials and plasticity. The research in this area is devoted to elastic materials with additional features that can be modeled in a quasistatic setting, including damage and crack propagation in elastic materials, which is jointly investigated with the Leibniz Group *Modeling of Damage Processes*. Another focus concerns elastoplasticity and phase transformations in shape-memory alloys, see also the Scientific Highlights article on page 39. These problems are treated in the MATHEON project C18 "Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys" and the project P5 "Regularizations and relaxations of time-continuous problems in plasticity" within the DFG Research Unit FOR 797 "Analysis and Computation of Microstructure in Finite Plasticity". A major achievement is the first global existence theory for energetic solutions for rate-independent gradient plasticity; see [5].

MICROPLAST

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

Regularity theory for partial differential equations. Many real-world applications involve partial differential equations on domains with nonsmooth coefficients and corners, so-called *heterostructures*, which are, e.g., common in semiconductor devices. In order to understand the properties of the solutions to such problems, it is crucial to know that the div-grad operator $\mathcal{A}_p : W^{1,p}_\Gamma(\Omega) \to W^{-1,p}_\Gamma(\Omega); u \mapsto -\nabla \cdot (\mu \nabla u)$ has a bounded inverse for some p greater than the space dimension. For "smooth constellations", the result holds for all $p > 1$, and Gröger [1989] showed that it always holds for $p \in]2-\delta, 2+\delta[$; however, δ is arbitrarily small in general.

Thus, in the most relevant, spatially three-dimensional case, one is still confronted with serious difficulties. The well-known obstructions to p-integrability are singularities of the solution in the

corners of the subdomains where the coefficients are constant. In [2], a characteristic function for the singularity exponents was derived in explicit form for multi-material edges (three or four materials), making it possible to show that $\mathcal{A}_p$ is an isomorphism for some $p > 3$ for three-dimensional model sets, which include, e.g., the benchmark L-shaped domain. This "toolbox of isomorphisms" gives access to the analysis of buried heterostructures in semiconductor devices and was applied successfully in optimal control for the thermistor problem.

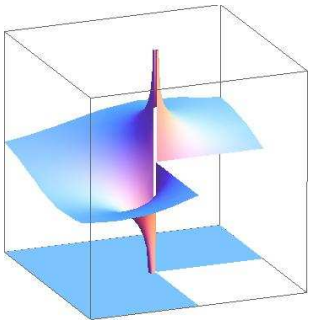


Fig. 2: *Corner singularity*

Quantum mechanics and operator theory. The increasing interest in modeling of electronic transport in nanowires drives the need for understanding the mathematical structures behind the corresponding quantum mechanical models. The absolutely continuous spectrum of the involved Schrödinger operators intrinsically relates to the electronic transport properties of the nanowires. In particular, to justify non-equilibrium steady states, one has to consider time-dependent families of self-adjoint extensions that converge, for $t \to -\infty$, to a Hamiltonian for noninteracting subsystems and to the full Hamiltonian for $t \to +\infty$. The problem is well-posed if the decoupled Hamiltonian has the same absolutely continuous spectrum as the full Hamiltonian or even if their absolutely continuous parts are unitarily equivalent.

In [6], the boundary-triplet approach was used to solve this problem. The results go beyond the usual assumptions in scattering theory, for the resolvent difference does not need to be of trace class. Under cylindrical symmetries, the symmetric and decoupled Hamiltonians decompose into an infinite direct sum of operators; see [7]. The method developed in [6] allows for an application to this situation and to strengthen the existing results, e.g., by avoiding compactness assumptions.

Numerical analysis for reaction-diffusion systems. In cooperation with the Research Group *Numerical Mathematics and Scientific Computing*, electro-reaction-diffusion systems were studied in order to find discretization schemes preserving the main features of the corresponding continuous problem, such as positivity of densities, balance of fluxes, conservation of energy, and increase of entropy. This could be achieved using a Voronoi finite-volume discretization and an implicit time-stepping scheme. Exponential decay to the discrete equilibria was established as well.

However, to obtain decay rates that are uniform for a family of refined Voronoi meshes, it was necessary to translate the quantities from the finite-dimensional discretized problems into expressions of functions defined on the continuous domain Ω. To this end, a discrete version of the classical Sobolev–Poincaré inequality $\|u - m_\Omega(u)\|_{L^q} \le c_q \|\nabla u\|_{L^2}$ was developed in [3], where the coefficient c_q is bounded uniformly along the refining sequence of Voronoi meshes. The proof of this result is based on a discrete form of Sobolev's integral representation and on estimating weakly singular integrals.

Halbleiter-Nanophotonik
SFB 787

Fig. 3: *SFB 797 (supported by DFG)*

Semiconductor modeling

This research group is involved in several projects related to nano- and optoelectronic devices. Together with Research Group *Laser Dynamics*, it runs the MATHEON project D14 "Nonlocal and nonlinear effects in fiber optics". The project B4 "Multi-dimensional modeling and simulation of VCSEL devices" within the DFG Collaborative Research Center (787) "Semiconductor Nanophotonics:

Materials, Models, Devices" is a collaboration with Research Groups *Laser Dynamics*, *Numerical Mathematics and Scientific Computing*, and the Zuse Institute Berlin (ZIB). We refer to the reports of these research groups for more information. In the following, we present several projects of the group that are ordered from small to large spacial scales.

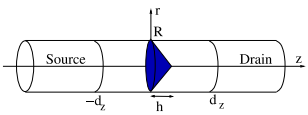


Fig. 4: *Conical quantum dot embedded into a nanowire*

Nanowire devices. The interest in nanowire-based devices has increased in the last years due to the very promising applications in nano-optoelectronics. The modeling of the electronic transport in nanowires with diameters of tens of nanometers has to be done on the quantum level. In contrast to electronic applications, for optical applications the main role is played by bound states. The formalism developed in [7] for computing the scattering states in cylindrical nanowire heterostructures makes it possible to consider the classically allowed energy levels corresponding to the continuous spectrum. The wave functions of the electrons for these energies are extended states, so-called *scattering states*. With these states it is possible to calculate electronic properties like the current through a nanowire.

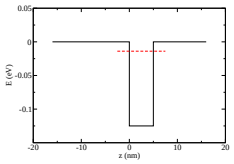


Fig. 5: *Energy of the bound state inside the conical quantum dot*

The classically forbidden spectrum contains the *bound states*, also called *localized states*. They are obtained with a proper choice of artificial boundaries for the Wigner–Eisenbud problem (see d_z in Figure 4) and correspond to lower energy levels. For Figure 5, the parameters for a conical quantum dot are chosen such that there is only one bound state. The corresponding Wigner–Eisenbud function yields the wave function Ψ of the bound states; see Figure 6 for a plot of $|\Psi|^2$.

Hence, this formalism can describe extended states as well as bound states of an electron scattered by a general potential in two dimensions. This general resonance theory shows that the two-dimensional character of the scattering potential and the strong coupling of the quantum system to the contacts allow for transmission profiles that range from asymmetric Fano-line shapes to "S-type" Fano lines to anti-resonances.

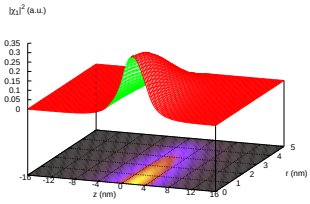


Fig. 6: *$|\Psi|^2$ for the bound state Ψ inside a conical quantum dot*

Further activities aim at including the effect of different effective masses in a heterostructure where the Wigner–Eisenbud problem has to be solved via finite elements. Another development considers the electron-electron interaction in the Hartree approximation by using the Schrödinger–Poisson system for nanowire heterostructures.

Kohn–Sham theory. To model nanoelectronic devices in which the electron-electron interaction is important, one uses the density functional theory, also called *Kohn–Sham theory*, describing a statistical ensemble of quantum mechanical, electrically charged, interacting particles. The aim is to find the particle density as a minimizer of the system's free energy. Apart from a fixed chemical potential energy of the background, the free energy consists of (i) the free energy of a reference system in thermodynamic equilibrium, (ii) the electrostatic interaction energy of the charged particles, and (iii) the exchange-correlation energy modeling the particle interactions. Neglecting the latter, the free energy is convex and has a unique minimum, while otherwise non-convexity leads to multiple critical points.

In [4], it was shown that the particle-density operator depends analytically on the chemical potential. This result is useful in bifurcation theory and for the construction of convergent iteration schemes that are studied in the MATHEON project D4 "Quantum mechanical and macroscopic mod-

els for optoelectronic devices". In order to comparatively evaluate these methods, a software tool based upon three-dimensional finite volumes was set up. A DIIS (Direct Inversion in the Iterative Subspace) acceleration scheme and underrelaxed fixed-point iterations have proved to be promising.

Additionally, a transient Kohn–Sham theory was developed as an abstract evolution equation of drift-diffusion type. The free energy decays along the solutions, and the stationary solutions are their critical points. The crucial steps in this approach are the analyticity and injectivity of the particle density [4] and a proper model of the current density including the mobility of particles.

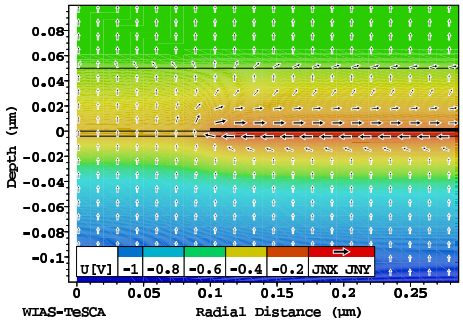


Fig. 7: *Current simulation in a thin-film solar cell using* `WIAS-TeSCA`

Photovoltaics. In the area of photovoltaics, the Research Groups *Partial Differential Equations* and *Numerical Mathematics and Scientific Computing* strengthened the cooperation with the relevant groups of the Helmholtz Center Berlin for Materials and Energy (HZB); see [1]. Moreover, together with several members of MATHEON, namely Volker Mehrmann (TU Berlin), Frank Schmidt (ZIB), and Barbara Wagner (RG 7), the group participates in the "Competence Center Thin-Film and Nanotechnology for Photovoltaics Berlin" (PVcomB), which is coordinated by HZB and financed by the Federal Ministry of Education and Research and the Federal State of Berlin for five years. The joint mathematical project is devoted to the analysis, modeling and simulation of optical and electronic properties of solar cells as well as the growth of thin films.

Fig. 8: *Herbert Gajewski*

Special events

On July 15, the celebration of ***Herbert Gajewski's*** seventieth birthday was held within the Berlin *Senior Seminar on Nonlinear Partial Differential Equations* (Langenbach Seminar). The scientific lecture was given by Professor Giuseppe Savaré, Università di Pavia, and was entitled *A Variational Approach to Gradient Flows in Metric-Measure Spaces*. The lecture connected the work of Gajewski on evolutionary problems with modern developments in the field. The following reception was well attended and gave ample time for recalling memories from the past and discussing science and other plans for the future.

Fig. 9: *Giuseppe Savaré*

Fig. 10: *Herbert Amann*

International Conference on Elliptic and Parabolic Equations. This conference took place at WIAS from November 30 through December 4, 2009. It was organized by Joachim Rehberg and Hans-Christoph Kaiser who were supported by the Scientific Board consisting of Monique Dauge (Rennes), Johannes Elschner (RG 4), Joachim Escher (Hannover), Eduard Feireisl (Prague), Konrad Gröger (Berlin), Matthias Hieber (Darmstadt), Grzegorz Karch (Wrocław), Dorothee Knees (LG 2), and Lutz Recke (HU Berlin).

Herbert Amann was the guest of honor and read a special lecture in the afternoon of December 2, 2009. There were 42 extended talks and several short communications and posters. Partial financial support by MATHEON is gratefully acknowledged.

Fig. 11: *EPE'09 participants*

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3.2 Research Group 2 "Laser Dynamics"

The research of this group is devoted to the development and application of mathematical methods and theories in the field of nonlinear dynamics. The main applied topics in 2009 were *dynamics of semiconductor lasers* and *pulses in nonlinear optical media*. The research related to these topics includes mathematical modeling, theoretical research on dynamical systems occurring in laser theory and nonlinear optics, numerical implementation, and device simulation.

An important event in the previous year was the International Workshop "Nonlinear Optics in Guided Geometries", May 18 – 20, organized together with G. Steinmeyer from Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy (MBI), Berlin. The workshop brought together leading international experts working both experimentally and theoretically in the fields of ultrashort optical pulses, femtosecond filamentation, pulse self-compression, solitons in photonic-crystal media, and optical dissipative solitons. In addition, the group organized two highly successful international minisymposia: "Dynamics of Coupled Phase Oscillators" (October 12) and "Nonlinear Dynamics in Quantum Dot Devices" (November 9).

Fig. 1: *Participants of the workshop "Nonlinear Optics in Guided Geometries"*

The group expanded their teaching activities through a lecture at Humboldt University (HU) of Berlin, in addition to their two traditional research seminars "Mathematical Photonics" and "Nonlinear Dynamics", organized together with HU and Free University (FU) of Berlin, respectively.

Uwe Bandelow completed his Habilitation and was a member of the Program Committee of NUSOD for its 2009 conference in Gwangju, South Korea. Andrei Vladimirov was a member of the Program Committee of the CLEO®/Europe-EQEC conference in Munich. Julia Ehrt successfully defended her Ph.D. thesis at FU Berlin.

Particular progress in the following fields of research should be mentioned:

Dynamics of semiconductor lasers

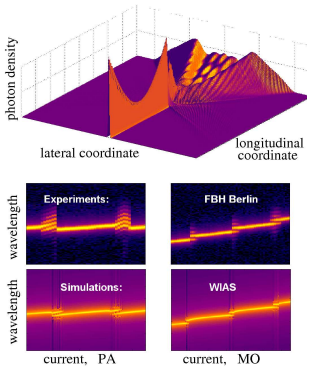

Fig. 2: *Top: a typical photon density distribution in a tapered Master Oscillator (MO) Power Amplifier (PA) laser. Bottom: dependence of optical spectra for increasing current injections*

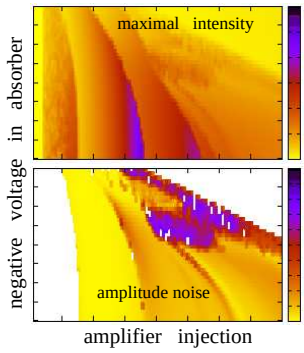

Fig. 3: *Characterization of a mode-locked quantum-dot laser in amplifier injection – absorber voltage plane. Top: maximal intensity of the emitted optical fields. Bottom: amplitude noise of the mode-locked pulsations*

In this main field of the group's applied research, existing models for the analysis of the effects in different types of semiconductor lasers were extended and used.

In particular, based on the spatially two-dimensional large-scale traveling wave model [1], the simulation and analysis of the dynamics of different *broad-area laser* structures was performed. Together with cooperation partners from the Ferdinand Braun Institute for High Frequency Technology (FBH), Berlin, the mode dynamics of high-power *tapered master-oscillator power-amplifier lasers* [1] were analyzed, followed by a parameter optimization study. The latter was possible in reasonable computation time because numerical algorithms for high performance parallel computing had been successfully implemented, tested, and calibrated on the new WIAS Euler compute cluster. In addition, jointly with colleagues from the Vilnius Gediminas Technical University (Lithuania), the group investigated the precision of several numerical schemes suited to simulate the related wave equation in infinite lateral domains.

After extending the underlying model, a *stripe-array diode laser* with delayed filtered optical feedback was analyzed. By changing the angle of the off-axis external feedback, one can control the global phase coupling of the stripe array. Thus, by supporting the natural in-phase operation of the stripe array, the laser could be stabilized to operate in a high-power anti-phase synchronized supermode with a high-power diffraction-limited output beam. The theoretical results were found to be in good agreement with previous experimental results from the University of Potsdam.

In project B5 "Effective models, simulation, and analysis of the dynamics in quantum dot devices" of the DFG Collaborative Research Center SFB 787 "Semiconductor Nanophotonics: Materials, Models, Devices" (jointly with Jürgen Sprekels, Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*), an efficient numerical scheme for modeling dynamical instabilities in monolithic passively mode-locked semiconductor lasers was proposed. This scheme was used to study bifurcation mechanisms of the development and break-up of different operation regimes in a *passively mode-locked monolithic semiconductor laser*. It was shown that mode-locking regimes with different repetition rates can be multistable for a wide range of laser parameters and that the harmonic mode-locking regime with two counterpropagating pulses in the cavity can exhibit a period-doubling bifurcation leading to different amplitudes and separations of the pulses.

Hybrid mode-locking in a monolithic quantum dot (QD) laser was studied theoretically using a set of five delay differential equations that take into account carrier exchange between quantum dots and the wetting layer. In cooperation with colleagues from Technical University (TU) of Berlin, a theoretical explanation of the experimentally observed strong asymmetry of the locking range with respect to the passive mode-locking frequency was obtained. The above-mentioned carrier exchange model was implemented in the group's software `LDSL-tool`. Other modifications of `LDSL-tool` comprise an arbitrary spatial dependence of the field coupling factor, allowing the simulation and analysis of *multicolor lasers*. Further features for data post-processing, e.g., for the plot of spectral mapping diagrams, were implemented.

The control of *unstable semiconductor lasers* was the topic of a cooperation with the University of

the Balearic Islands (Palma, Spain) and the Free University of Brussels. The advantages of controlling the unstable dynamics of a semiconductor laser subject to conventional optical feedback by means of a second filtered feedback branch were demonstrated in [2]. An overview of the analytical solutions in the case of double cavity feedback was provided. It was shown that the region of stabilization can be increased using a second branch with filtered rather than conventional feedback.

Further, the fruitful collaboration with Klaus Gärtner and Thomas Koprucki from the Research Group *Numerical Mathematics and Scientific Computing*, and with Andreas Knorr from TU Berlin, within project B4 "Multi-dimensional modeling and simulation of VCSEL devices" in the framework of the DFG Collaborative Research Center SFB 787 "Semiconductor Nanophotonics: Materials, Models, Devices" (jointly with Alexander Mielke, Research Group *Partial Differential Equations*, and Frank Schmidt, Zuse Institute Berlin), should be mentioned. The activities concentrated on mathematical and numerical modeling, in particular on the efficient coupling of the optical with the electrical model and, with respect to the latter, on the integration of quantum structures into the spatially resolved transport model.

Pulses in nonlinear optical media

Within project D14 "Nonlocal and nonlinear effects in fiber optics" of the DFG Research Center MATHEON, a nonlocal pseudodifferential dispersion operator was introduced that yields an adequate description of arbitrary medium dispersion and absorption in a wide spectral region. On this basis, both envelope and non-envelope models for pulse propagation were formulated and investigated. These models correctly describe the dynamics of few-cycle and even sub-cycle optical pulses. Furthermore, a Hamiltonian framework for ultrashort optical pulses propagating in nonlinear fibers was developed. Unidirectional propagation equations were derived using classical analogues of quantum creation and annihilation operators. The Hamiltonian formulation directly provides integrals of motion that are related to the averaged fluxes of energy, momentum, and photon number along the fiber. These integrals were used to control the quality of numerical solutions. In addition, localized solutions of propagation equations were derived by constrained minimization of the Hamiltonian. This technique offers a simple way to calculate ultrashort optical solitons for arbitrary dispersion and examine their stability.

In the DFG project "Pulse shaping in hollow-fiber compressors: Simulation and experiment", including experiments at Max Born Institute, filamentary propagation was investigated. The group's joint research with MBI on the propagation of short pulses in a filament shed new light on the rather surprising effect of self-compression, namely the formation of short pulses occurring in two separate steps [3], and involving a self-pinching mechanism similar to the z-pinch contraction of pulsed high-current discharges.

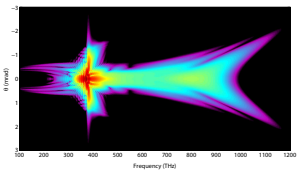

Fig. 4: *Angularly resolved far-field spectrum of a double self-compressed femtosecond pulse in a laser filament, exhibiting the generation of hyperbolic shock waves*

Furthermore, together with colleagues from the Université Libre de Bruxelles and the Imperial College London, properties of two-dimensional cavity solitons in a coherently driven optical resonator subjected to delayed feedback were investigated [4]. The delay was found to induce a spontaneous motion of a single cavity soliton that is otherwise stationary and stable. This behavior occurs when the product of delay time and feedback strength exceeds some critical value. An analytical descrip-

tion of the transition from a stationary to a moving soliton was provided, which agrees with the results of the group's numerical simulations.

Dynamical systems

Concerning the topic of delay differential equations (DDEs), a major breakthrough was the rigorous proof of a complete asymptotic description of the spectrum of fixed points in the singular limit of large delay [5]. In this limit, the spectrum separates into a point spectrum and a critical pseudo-continous spectrum, which—after a rescaling—is located on curves. Asymptotic approximations of both parts of the spectrum can be deduced from the coefficients of the DDE, independently of the delay parameter.

In collaboration with colleagues from the Université Libre de Bruxells and the Lille University of Science and Technology, beating between two intrinsic frequencies generated simultaneously by modulation (Turing) instability was analyzed in the driven-damped nonlinear Schrödinger equation, which describes a coherently driven photonic crystal fiber cavity [6]. Beating in the form of a slow modulation of fast intensity oscillations was found to be stable for a wide range of parameters. It was shown that this beating can form localized structures that contain only a finite number of slow modulations. Such structures consist of dips in the amplitude of the fast intensity oscillations, which can either be isolated or regularly spaced. The asymptotic analysis close to the modulation instability threshold makes it possible to interpret this phenomenon as a manifestation of homoclinic snaking for dissipative localized structures.

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3.3 Research Group 3 "Numerical Mathematics and Scientific Computing"

The research activities of the group concentrated on the development, study, and application of numerical methods for partial differential equations (PDEs) and differential-algebraic equations (DAEs). Finite volume methods and finite element methods are the basis of the numerical schemes. Special emphasis is paid to conservation properties of the schemes. The applications considered include simulations of semiconductor devices, see the Scientific Highlights article on page 24, electrochemical reactions, see the article on page 49, processes in gas turbines, and particulate flows. There exists an intensive collaboration with Leibniz Group 1.

Mesh generation

The research focused on algorithms for the generation of three-dimensional boundary-conforming Delaunay meshes that are necessary for the implementation of the Voronoi box based finite volume method. This method is used extensively in simulations of semiconductor and electrochemical devices performed in the group. The mesh generator `TetGen` has been developed in this project. New results in the analysis of one of `TetGen`'s key algorithms were achieved in [6].

In 2009, there was a new release of `TetGen`, version 1.4.3. It contains several major improvements in the algorithms and implementations that enhance the performance and stability of the program. Meanwhile, `TetGen` is well established on the international level. A number of cooperation and license requests created options for future collaborations.

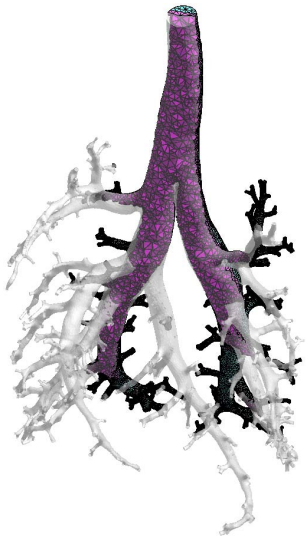


Fig. 1: *A view of a tetrahedral mesh of a rat lung generated by* `TetGen` *(PNL, USA)*

Post exposure bake in photolithography

The group participates in the Specific Targeted Research Project MD^3 „Material Development for Double Patterning and Double Exposure" funded by the European Commission within its 7th framework program. The aim of this project is to evaluate strategies for the creation of 32 nm structures using current optical techniques based on lenses.

Photolithography is an essential step during the manufacturing of semiconductor devices. It starts with depositing a photoresist polymer layer on top of a semiconductor wafer and exposing certain parts of it to light, generating acid molecules. At elevated temperatures, in the following post-exposure-bake step—which can be modeled by a system of reaction-diffusion equations—these acid molecules break polymer crosslinks, allowing the selective removal of the resist in a subsequent process step called *development*. The current exposure technology is based on optical lenses. The resolution of this process is thus limited by the wavelength of visible light. Double patterning using a litho-freeze-litho-etch (LFLE) process is one option to remove this barrier. Here, after freezing the resist remaining from the initial process, a secondary resist is deposited, exposed, baked, and developed. Interactions between the primary and secondary resists may influence the final structure. In particular, photogenerated acid may diffuse from the secondary to the primary

resist, becoming unable to break crosslinks in the secondary resist. This may be an explanation for the experimentally observed resist "footing", i.e. secondary resist remaining in the vicinity of the primary resist; see [1] and Figure 2.

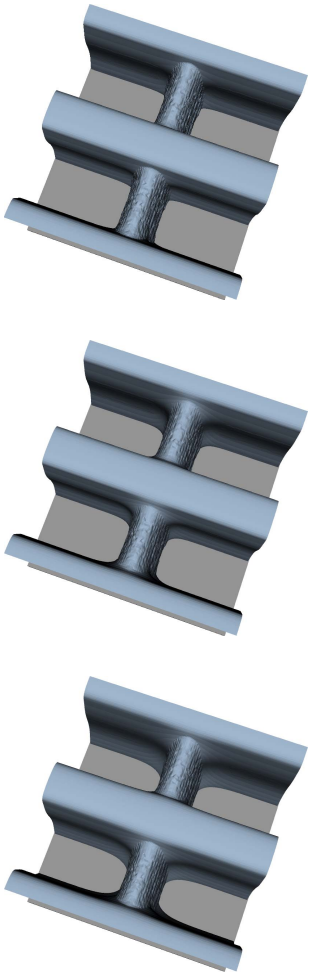


Fig. 2: *Cross-line configurations after a double patterning process for different combinations of acid diffusion lengths in the primary and secondary resist. Primary (thick) resist lines span from top left to bottom right, while secondary (thinner) structures are orthogonal to them and exhibit increasing width and footing with increasing acid diffusion length.*

Using the Voronoi box based finite volume method, and its ability to work on a large class of geometries, the group created the WIAS–PEB module for the numerical simulation of the post-exposure-bake step over a given topology, as it occurs in the LFLE approach. As planned for the project, this module contributes to the process simulation tool box "Dr. LiTHO" (Fraunhofer Institute of Integrated Systems and Device Technology (IISB), Erlangen), where it can be used together with tools modeling exposure and development steps.

Process simulation for gas turbines

The block-oriented process simulator BOP, which is developed and maintained by the group, has been designed to solve large-scale process simulation problems. The simulation concept is characterized by the integration of a BOP compiler that directly generates an appropriate system of DAEs out of the industrial process description, by the implementation of divide-and-conquer techniques, and by the combination of deterministic and stochastic numerical methods.

For a couple of years, the main industrial application area of BOP has been the simulation of heavy-duty gas turbines for power plants. Based on a long-term cooperation and support agreement valid until 2014, BOP is licensed to ALSTOM Power Ltd., a global leader on the world market of power generation. In 2009, version BOP2.5 was delivered to ALSTOM. Now BOP covers the entire relevant work process applied in ALSTOM's gas turbine performance development from basic design data computation to heat balance evaluation to stochastic analysis.

Version BOP2.6 is under development, and is going to be delivered in 2010. Apart from other improvements, this version provides a converter between an industrial standard language and the modeling language MLBOP, a homotopy mode for the simulation of carbon dioxide refeeding, and an optimization mode based on Monte Carlo data. In future, the optimization mode of BOP will be extended to general inverse optimization tasks resulting from model calibration problems. An enhancement of the BOP compiler supporting a "cycle modeling tool" is under development.

Variational multiscale methods for the simulation of incompressible turbulent flows

Variational multiscale (VMS) methods are a rather new approach for turbulent flow simulations. Similarly to the popular large eddy simulation (LES), only large scales of turbulent flows are simulated. In contrast to LES, the scales are not defined by spatial averaging (filtering) but via projections into appropriate function spaces. This definition avoids some difficulties of LES methods, such as commutation errors.

A three-level finite element VMS method with explicit projection has been developed and studied for a couple of years. This method uses a decomposition of the resolved scales into large and resolved small scales. The direct influence of the turbulence model on the impact of the unresolved

scales is confined to the resolved large scales. The scale separation requires an additional tensor-valued finite element space L^H for the large scales. In a number of numerical studies published in the preceding years, L^H was chosen before the simulations such that the same local finite element was used for all mesh cells.

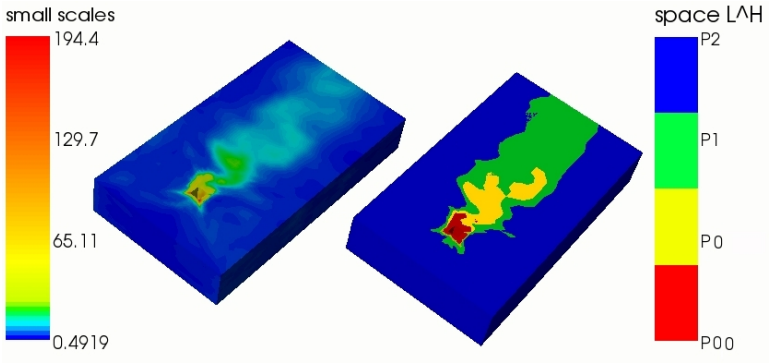


Fig. 3: *Turbulent flow around a cylinder with square cross section at* $\mathrm{Re} = 22\,000$. *Snapshot of the indicator of the turbulent intensity (left) and the resulting space* L^H; *P00 – local space only consists of the zero tensor; from [2]*

An extension of this approach allowing the computation of L^H during the simulations with the possibility of different local finite elements in different mesh cells was presented in [2]. In very turbulent subregions of the flow, the turbulence model has to have a large influence. This can be a posteriori controlled by using locally a small space L^H. Likewise, in laminar subregions, a larger space L^H is used, and the turbulence model may even be switched off. The choice of the local space L^H is controlled by the size of the computed local resolved small scales. To the group's best knowledge, this is the first VMS method with an adaptively chosen large scale space.

Numerical studies considering a turbulent channel flow and a turbulent flow around a cylinder on hexahedral meshes are presented in [2]. Figure 3 shows a snapshot of the size of the resolved small scales and the resulting space L^H. The local turbulent intensity is large at the cylinder and the local space L^H consists just of the zero tensor. Away from the cylinder, much less turbulence occurs such that a small influence of the turbulence model suffices and L^H can be chosen larger. The numerical studies show some improvement compared to the static choice of the large-scale space.

This method was extended to tetrahedral meshes for the $P_2^{\text{bubble}}/P_1^{\text{disc}}$ finite element in [3]. Tetrahedral meshes are necessary for complicated domains. Figure 4 shows the size of the resolved small scales in a reactor geometry with torispherical head, two inlets at the top, and an outlet on the bottom. It can be observed that the regions with high turbulence intensity and the regions without turbulence are predicted correctly.

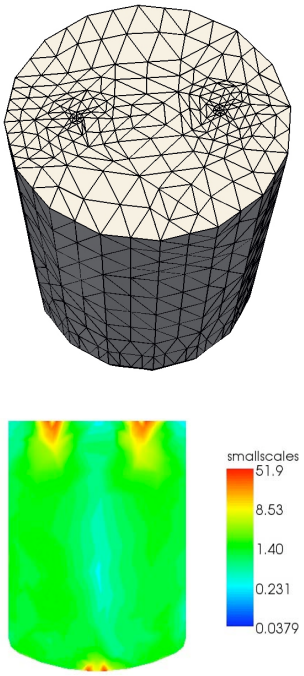


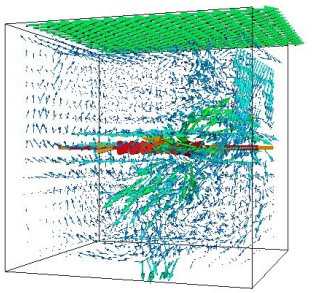
Fig. 4: *Reactor with torispherical head, grid (generated with* `TetGen`*), and magnitude of the resolved small scales in the cut plane with the inlets; from [3]*

Simulation of population balance systems

Population balance systems model the transport of particulate species in fluids. These consist of a coupled system of Navier–Stokes equations (flow field), convection-dominated convection-diffusion-reaction equations (temperature, concentrations, chemical reactions), and an integro-

partial differential equation (particle size distribution, PSD). A main challenge in the simulation of such systems comes from the fact that the PSD does not only depend on time and space, like the other functions in the system, but also on properties of the particles, the so-called *internal coordinates*. Consequently, population balance systems couple equations that are defined in domains with different dimensions.

The main focus of the research was on appropriate schemes for the higher-dimensional transport equation for the PSD (yet without integral terms) modeling a calcium carbonate precipitation. Numerical studies [4, 5] show that different numerical schemes lead to qualitatively different results for an output of interest, in particular in the presence of highly unsteady flows. First simulations of a calcium carbonate precipitation in a turbulent flow field were presented in [5]. The finite element VMS method was used as turbulence model in these simulations.



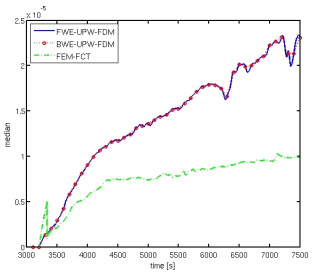


Fig. 5: *Turbulent flow in a cavity with two opposite inlets and an outlet, velocity field and median of the volume fraction at the outlet for the precipitated calcium carbonate, computed with different numerical schemes; from [5]*

Software environment for the numerical solution of partial differential equations

The software environment `pdelib2` provides a framework for integrating the different stages of numerical algorithms' development, like mesh generation, numerical solution, and visualization. It is used in a number of WIAS projects, e.g., the heat treatment of steel, simulations of milling processes (both in collaboration with Research Group 4), electrochemical modeling (with Leibniz Group 1), and post exposure bake in photolithography. In addition, a test environment that protects critical features was introduced. The script binding interface for finite element computation was extended, especially with respect to its use in optimal control problems governed by PDEs. Furthermore, the interface allows the registration of block assembling operators for coupled systems from user projects. A new module for time integration of stiff and nonstiff ODE systems was developed. S-stage implicit and explicit Runge–Kutta methods with the Butcher diagrams as input and extrapolation methods were implemented, which were derived from abstract base classes.

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3.4 Research Group 4 "Nonlinear Optimization and Inverse Problems"

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

Part of the research is carried out within the projects B20, C7, and C11 of the DFG Research Center MATHEON and within two projects in the DFG Priority Programs SPP 1180 and SPP 1204, respectively (see page 100). The group took part in the Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", supervising two Ph.D. projects.

In 2009, the group further extended its successful collaboration with industry and partners from the engineering sciences. Its expertise in stochastic optimization led to the participation in a funded project with a leading natural gas transmission company. Research carried out within the DFG Priority Program SPP 1204 related to the inverse problem of detecting phase transition kinetics from measurements aroused the interest of a dilatometer manufacturer and paved the way to a joint two-year project funded by the Central Innovation Program for Small and Medium-sized Enterprises (ZIM) of the Federal Ministry of Economics and Technology.

A special event was the colloquium on the occasion of Johannes Elschner's 60th birthday. George Hsiao (University of Delaware), Gunther Schmidt (RG 4), Reinhold Schneider (Technical University of Berlin), and Masahiro Yamamoto (University of Tokyo) reported on recent results in inverse problems, integral equations, and variational analysis of PDEs. In these areas Johannes Elschner has made significant contributions, which in 2009 also led to a new DFG individual grant project on direct and inverse problems for elastic waves.

In the sequel, scientific achievements of the research group in 2009 are detailed.

Optimization and optimal control

The research in stochastic optimization was driven by problems arising within MATHEON project C7 "Mean-risk models for electricity portfolio management and stochastic programming". Progress was made in three directions: first, theoretical and algorithmic work on scenario reduction for mixed integer stochastic optimization problems was completed. Secondly, a numerical method for solving joint probabilistic constraints was implemented and applied to case studies in hydropower management (see Figure 1). This topic is closely related to a project funded by Electricité de France (EDF). Finally, research on explicit stationarity conditions for electricity spot market models was continued. A Ph.D. thesis supervised in GRK 1128 focussing on theoretical aspects of this subject was completed and submitted. An important result in this context is the investigation of transformation formulae for the Mordukhovich coderivative, provided in [5]. The expertise in stochastic programming led to the participation in the recently initiated new MATHEON project B20 "Optimization of gas transport".

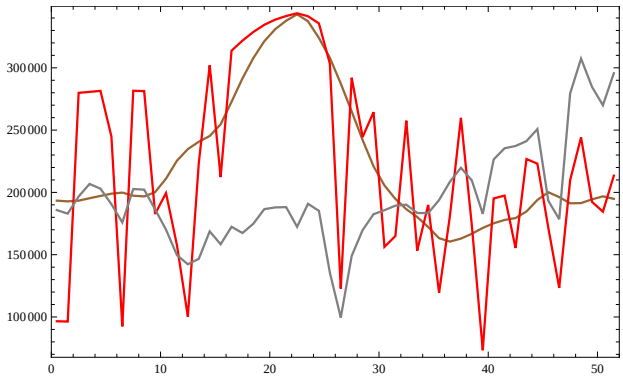

Fig. 1: *Optimal release policy (red) in hydro-power management (one year, weekly decisions). Mean inflows to the reservoir (brown) and mean prices for sale of electricity (gray) are additionally plotted*

In PDE-constrained optimal control, research regarding error estimates for state-constrained control problems was continued. In collaboration with Christian Meyer (Technical University of Darmstadt) and Arnd Rösch (University of Duisburg-Essen), a priori finite element error estimates for state- and control-constrained Neumann boundary control problems were investigated [7]. The purely state-constrained problems are regularized with the so-called *virtual control concept*. Then, the arising problems are discretized by linear finite elements for the state and the boundary control. Errors induced by the regularization and the discretization were simultaneously studied using an appropriate coupling of the respective parameters.

In a joint study with Ira Neitzel (Technical University of Berlin) and Arnd Rösch, a class of semilinear elliptic optimal control problems with pointwise state and control constraints was studied. Assuming a sufficient second-order optimality condition and uniqueness of the dual variables, it could be shown that the second-order sufficient optimality condition can be carried over to regularized versions of the original problems, provided that the regularization parameter is chosen sufficiently small. Moreover, error estimates with respect to the regularization parameter were derived.

In MATHEON project C11 "Modeling and optimization of phase transitions in steel", the focus lay on the study of distortion compensation by optimizing the final phase mixture. To this end, optimality conditions for the resulting state system were investigated. A great deal of work was done as well on the implementation of optimization strategies for this challenging multi-field problem within `pdelib` (see Figure 2).

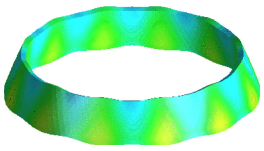

Fig. 2: *Temperature and displacement during cooling of a conical ring*

In continuation of the work regarding control of Joule heating [6], a coupling with a nonsmooth phase field equation to model phase transitions triggered by heating was studied jointly with Elisabetta Rocca (University of Milan). In a first step, existence and uniqueness results were derived, which will be later applied for the study of related control problems.

Inverse problems

The focus of research in the project "Simulation and control of phase transitions and mechanical properties during hot-rolling of multiphase steel" within DFG SPP 1204 in 2009 lay on numerical methods for the identification of phase transition laws from dilatometer measurements. A special feature was the consideration of increased nucleation due to the rolling and the redistribution of carbon. In a joint work with Jijun Liu (Southeast University, Nanjing), numerical methods for an

efficient numerical solution to the related identification problem were developed. Further studies centered around the parameter identification of an experimental hot-rolling mill at the Freiberg University of Mining and Technology. Thus, all prerequisites for the ultimate goal to optimally control the cooling section in a real hot-rolling mill are provided.

One objective of the new DFG individual grant project "Direct and inverse scattering problems for elastic waves" is to develop a new solvability theory for direct elastic scattering problems based on variational formulations. In this respect, diffractive structures with nonsmooth interfaces and several elastic materials are of particular interest. In [1], this goal was successfully achieved for the scattering of time-harmonic plane elastic waves by a two-dimensional periodic structure (diffraction grating). In the case of an impenetrable interface, the grating profile is given by a Lipschitz curve on which the displacement vanishes (Dirichlet problem). Using a variational formulation in a bounded periodic cell involving a nonlocal boundary operator, existence of solutions in quasi-periodic Sobolev spaces could be proved by establishing the strong ellipticity of the corresponding sesquilinear form. Moreover, uniqueness in the Dirichlet problem was shown under the assumption that the grating profile is given by a Lipschitz graph. The variational approach was extended to the practically important case of transmission gratings where several homogeneous elastic media are separated by periodic Lipschitz interfaces.

The inverse scattering problem of determining a bounded obstacle by its far-field pattern is fundamental for exploring bodies by acoustic, electromagnetic, or elastic waves. Establishing the uniqueness in this inverse problem by using the far-field data from only one or, at most, finitely many incident plane waves remains a challenging open problem. Recent progress in this direction was obtained in inverse acoustic and electromagnetic scattering by polyhedral scatterers. Continuing the cooperation with Masahiro Yamamoto (University of Tokyo), the third and fourth exterior boundary value problems of linear elasticity were studied. First uniqueness results for the corresponding inverse scattering problems with polyhedral-type obstacles and a finite number of incident plane elastic waves [2] could be obtained using a new reflection principle for the Navier equation.

The cooperation with the Physikalisch-Technische Bundesanstalt (PTB) on inverse problems for the scatterometric measurement of photolithographic masks continued in the framework of the BMBF project "CDuR 32". The impact of model parameter and measurement uncertainties on the reconstruction was analyzed with Monte Carlo procedures in [4]. These simulations revealed that the reconstructed values for side-wall angles and critical dimensions (lateral widths) depend strongly on the underlying multilayer system. Therefore, the two-dimensional code was extended to include parameters of the multilayer system into the sets of optimization parameters for the inverse algorithm. The implemented computation of the corresponding Jacobians results in linear approximations of the covariance matrices and estimates for the uncertainties. The development of a three-dimensional reconstruction algorithm was also continued. For the simulation step, a typical class of test structures for the EUV scatterometry for biperiodic gratings was implemented. The optimization algorithms rely heavily on the computation of the derivatives with respect to the geometry parameters (shape derivatives). To treat the case of conical diffraction by piecewise smooth two-dimensional structures, the field equations were considered in weighted Sobolev spaces. Using these results, shape derivative formulas for transmission curves with corners were derived.

In cooperation with colleagues from the Paul Drude Institute for Solid State Electronics (PDI), the light illumination of nano-wire arrays was studied. Experiments demonstrate that light is generated at a wavelength that is different from the one of the illuminating light. In order to quantify this radiation, the absorption of light in the wires was computed. Numerical tests show higher rates of absorptions on wire arrays than on bulk materials.

The work on analytic properties of integral formulations for conical diffraction, the development of numerical algorithms for multilayer gratings and their implementation was also continued in 2009 (see Figure 3). Details regarding modeling and analysis can be found in the Scientific Highlights article "Conical Diffraction" by Gunther Schmidt on page 54.

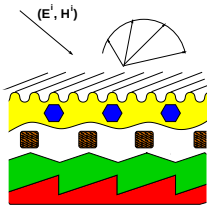

Fig. 3: *Multilayer grating with inclusions*

For multilayer gratings with inclusions a marching algorithm was developed that is based on the scattering matrix approach and allows to simulate classical and conical diffraction for gratings with an arbitrary number of layers separated by piecewise smooth interfaces. This algorithm was implemented within the framework of a cooperation with the International Intellectual Group, Inc. (Staten Island), on consultation and software development for conical diffraction problems. For details about the basic algorithm and results for actual engineering problems the reader is referred to [3].

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3.5 Research Group 5 "Interacting Random Systems"

After Anton Bovier and most of the members of the research group had left WIAS in 2008, the stochastics group became rather small, but nonetheless stayed very active. In fall 2009, the new head, Wolfgang König, arrived from the University of Leipzig, and with him two new postdocs, Sabine Jansen from the Princeton University and Bernd Metzger from the Université Paris 13. This was the beginning of a new group, whose goals are not much different from those of the former. With new forces, the group continues to study large systems with random input, defined on microscopic scales, and to describe the behavior of the system on mesoscopic and macroscopic scales. The methods employed are combinations of probabilistic and analytic tools, such as large deviations, stochastic differential equations, and martingales, as well as variational analysis, partial differential equations, and convex analysis. Various applications are considered, including fluent gases, Bose gases at positive temperature, large financial markets, random transport through random media, and interacting random walks.

Even though the year 2009 had an intermediate character for the research group, a couple of promising and well-earned successes can be reported. As a result of the work in the MATHEON project with his advisor Anton Bovier (now Bonn), Alexander Weiß received his Ph.D. in mathematics from the Technical University of Berlin in fall 2009 and temporarily completed his research on the optimal execution of large orders. Wolfgang Wagner continued his internationally highly regarded work on coagulation and fragmentation processes and received some prestiguous invitations. Alessandra Bianchi completed an impressive work [1] on metastability via coupling in collaboration with Anton Bovier and Dmitry Ioffe (Haifa) and left WIAS in fall 2009 to begin a new postdoc position at the University of Bologna. Bernd Metzger finished a nice piece of work together with Prof. Frédéric Klopp (Paris) on condensation phenomena in a random medium. Together with his collaborators from England and Italy, Wolfgang König described the cloud sizes in large classical dilute interacting point systems in the thermodynamical limit; some deeper work on the transition between different degrees of diluteness is going on at WIAS with Bernd Metzger and Sabine Jansen.

There is also some positive news about third-party funding. The DFG Research Unit FOR718 *Analysis and Stochastics in Complex Physical Systems* was extended by DFG for three more years and began its continuation at WIAS in fall 2009. This group, together with two postdoc positions, is now based at WIAS and is equipped with funds for guests, travel, and workshops for its members at Technical University of Berlin and the universities in Leipzig, Bonn, and Heidelberg.

In what follows, some of the highlights of the scientific work of the group in 2009 are detailed.

Coagulation and fragmentation processes

Coagulation and fragmentation processes occur in many sciences and application areas where objects of various nature can stick together or break into pieces. Kinetic equations are a common deterministic tool for describing the behavior of the size distribution of those objects. On the other hand, random particle models can be used for both analytical studies and numerical purposes.

Further progress was achieved in the development of efficient numerical algorithms for problems arising in the area of chemical engineering. The formation of soot particles in combustion systems is a highly complex process, which calls for detailed modeling of the resulting soot particle populations.

Fig. 1: *Soot aggregate*

Stochastic population balance methods allow for arbitrarily complex models of individual particles to be included with little additional impact on computation times. Coupling between stochastic particle population balance methods and stiff differential equation solvers used to treat chemically reacting systems is a particularly challenging problem, because of the different natures of the two solution methods. Several new results were obtained in collaboration with the Department of Chemical Engineering and Biotechnology (University of Cambridge, UK). In particular, a robust and less computationally demanding operator splitting method was proposed in [2].

A specific phase transition occurs in the context of fragmentation models when the fragmentation rate grows sufficiently fast at zero, leading to the formation of "zero-size particles" called "dust". On the analytical side, one observes that there exist nonconservative solutions to the general multiple fragmentation equation. On the side of stochastic models, the transformation into dust corresponds to the explosion phenomenon, that is, the accumulation of infinitely many jumps on a finite time interval. Based on general criteria introduced in an earlier work of the group, explosion properties of two random fragmentation models are studied in [5]. The sufficient conditions in terms of the kinetic coefficients are compared to results previously obtained, either by analytical tools, or by stochastic methods for the specific class of homogeneous random fragmentation models.

Interacting Bose systems

Predicted by Satyendra Nath Bose and Albert Einstein in 1924–25 in the context of noninteracting, identical particles with integer spin, now known as bosons, Bose–Einstein condensation (BEC) was experimentally realized only seventy years later: at temperatures very near to absolute zero, a large fraction of the bosons occupy the lowest quantum state, and quantum effects become apparent on a macroscopic scale. Obtaining this condensation phenomenon is a difficult problem, due to naturally arising interaction effects and due to the extremely deep temperatures that are required. Based on the attempt to understand this phenomenon theoretically, real Bose gases as well as idealizations like the Bose–Hubbard model have become paradigmatic objects in the study of interacting systems and related (quantum) phase transitions.

One line of research is the mean-field approach to Bose systems via the Gross–Pitaevskii approximation, where interaction effects are encoded in a nonlinear energy term competing with the quantum mechanical one-particle energy. One problem in this setting is the transfer of the notion of BEC to the interacting regime. Assuming, for example, a random background potential, an analog of classical BEC as well as new phenomena, like fragmented BEC or Lifshits glasses, are expected. The rigorous mathematical analysis of these problems is partially done in [4], nevertheless further research is necessary.

Phase transitions for classical interacting point systems

The description of large point systems with mutual short-distance repellence and medium-distance attraction is usually modeled with the help of an pair-interaction potential of Lennard–Jones type. The group studies the behavior in large boxes such that the particle density vanishes as the box increases with the particle number, i.e., dilute systems, at positive but vanishing temperature. Of particular interest is the question whether the system develops certain structures like crystals at some positive density and how large and how frequent these structures are.

In [3], the behavior in the thermodynamic limit is expressed in terms of an explicit variational formula, whose analysis shows that the point system arranges itself in a large number of clusters of just one size, which itself depends on the value of the temperature parameter. The clusters are widely spread in space, and their inner geometry approaches a certain deterministic optimal shape. The optimal size jumps at certain transition points on the temperature scale, and there are extreme phases with singletons and with infinitely large clusters, respectively.

The sharp concentration in clusters of just one size is a phenomenon that seems to occur only in dilute cold systems. Future work will be done on the regime of fixed positive temperature and particle density and the transitions to dilute cold systems, but this seems to require much deeper research.

The optimal execution of large orders

A recent problem of financial mathematics is the question for optimal strategies to execute large orders. Large orders are purchases or disposals of a number of shares that exceeds the offered supply at the best price. If executed immediately, large orders consequently induce a price impact that is undesirable for the executing trader. Yet, if the trader has a certain span to complete the execution, he or she can split the order into smaller pieces and trade them successively. Between two consecutive trades, the trader is inactive such that the market has time to recover. The question is how to split the large order and how to choose the execution times within the given time interval to minimize the negative price impact.

The optimal strategy depends on the assumptions about how the market recovers from a large order. It is generally difficult or even impossible to check the assumptions' validity in real markets. Instead, a microscopic market model can serve as an artificial trading environment to test trading strategies. Even if an artificial market environment cannot simulate the whole complexity of real markets, it can reveal oversimplified assumptions on a qualitative level.

In particular, Alfonsi, Fruth, and Schied (AFS) recently proposed a market model and proved that, for a given set of market parameters, there is a unique optimal strategy for this model, which is explicitly computable. A crucial assumption of this model is the existence of a constant that describes the recovery speed of the market. The group used the "opinion game", a microscopic market model introduced by Bovier, Černý, and Hryniv in 2006, to test the optimal strategies of the AFS model. The simulations showed that the recovery speed of the market in the opinion game is not sufficiently described by a constant, but is a function of the volume of the executed order.

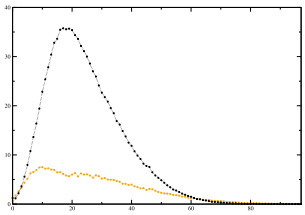

Fig. 2: *The empirical average of the supply of sell orders in the opinion game's order book. The x-axis denotes the prices relative to the best ask price. The orange graph illustrates the standard deviation.*

In [6], the group proposes a generalization of the AFS model incorporating the particular dependency. Then, the existence of unique strategies is proved, which are again explicitly computable. In addition, further assumptions of the ASF model are highlighted that are questionable.

These observations point out what more general market models could look like. The investigation of these enhanced models is a current research subject and is carried out in close cooperation with the Research Group *Stochastic Algorithms and Nonparametric Statistics*.

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3.6 Research Group 6 "Stochastic Algorithms and Nonparametric Statistics"

The research of the group is organized in the research projects Statistical Data Analysis and Applied Mathematical Finance. The focus is on applications in economics, financial engineering, life sciences, and mathematical physics. Of special interest are the modeling of complex systems using methods from nonparametric statistics, statistical learning, risk assessment, and valuation in financial markets using efficient stochastic algorithms and various tools from classical, stochastic, and rough path analysis.

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 two MATHEON projects A3 and E5 and the SFB 649 projects B5 and B7 (see page 99). Members of the group were involved in several industrial contracts. The existing collaborations with Landesbank AG on new pricing methods for Bermudan products and the collaboration with HSH Nordbank on pricing and calibration of different financial instruments was continued. The group also participates in a contract with ALSTOM (Switzerland) Ltd., on "Gas turbine process simulation". The contribution concentrates on general statistical modeling and Monte Carlo approximations.

Scientific highlights achieved by the research group in 2009 are provided below.

Statistical data analysis

The focus within the project area Statistical Data Analysis is on methods that automatically adapt to unknown structures using some weak qualitative assumptions. This includes, e.g., methods for dimension reduction, multiple testing, signal detection, feature identification, and adaptive smoothing.

Highlights 2009:

- EU project MASH, 2 Ph.D. positions for 2010–2012 (see page 84)
- Leibniz Association, *Pact for Research and Innovation*: project with Deutsches Diabetes-Zentrum Düsseldorf (DDZ), 1 Ph.D. for 2010–2012
- Leibniz Association, *Pact for Research and Innovation*: project with Potsdam Institute for Climate Impact Research (PIK), 0.5 Ph.D. for 2010–2012
- Ph.D.: Elmar Diederichs at Free University of Berlin, supervision: Vladimir Spokoiny
- Workshop on Structure Adaptive Methods, WIAS, November 6–8, 2009
- Compact courses on Modern Nonparametric Statistics held in Rennes (France) and Yale (USA) by Vladimir Spokoiny.

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

Statistical methods for imaging and neuroscience applications have been implemented within the R-Project for Statistical Computing. The corresponding packages are now part of the Medical Image Analysis task view within *The Comprehensive R Archive Network (CRAN)* and have been accepted by the *Neuroimaging Informatics Tools and Resources Clearinghouse (NITRC)*.

In statistical applications, there is an increasing interest in problems with high-dimensional observations, often with sample size in the same range or even smaller than the dimensionality of the data. Successful modeling heavily relies upon sparsity, i.e. identification of low-dimensional subspaces containing the data. The research group developed several methods, e.g., non-Gaussian component analysis (NGCA), sparse (SNGCA) [7], and adaptive methods for multi-index models. These methods offer new approaches to signal extraction, signal identification, and regression modeling, including applications to high-dimensional risk management.

The problem of simultaneous testing of a large number of statistical hypotheses, a topic with long-standing historical roots in statistics, recently enjoyed a significant surge of interest due to a large demand from numerous application fields (for example, bioinformatics and computational chemistry). The research on this area within the group addresses modern challenges. In particular, the group focuses on the design of testing procedures that can deal with a large body of data in possibly very high dimension, while maintaining a robust and accurate control of the type I errors (as measured by different standard criteria such as the family-wise error rate of the false discovery rate). For practical relevance, this control has to be valid in a nonasymptotic regime. Furthermore, the group concentrates on the design of procedures that are adaptive with respect to unknown nuisance parameters, such as the dependence structure between the testing statistics of different hypotheses, the proportion of false null hypotheses in the pool of hypotheses to test, and the alternative distribution. In particular, resampling procedures with a nonasymptotical error control are studied to this end. The publishing of a general-purpose open multiple testing toolbox (in the statistical language R) is planned for early 2010 in cooperation with the Technical University (TU) of Berlin, with funding from the European network PASCAL2.

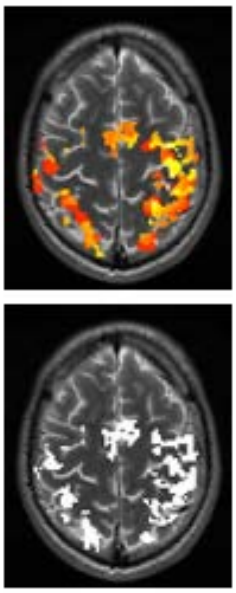

Fig. 1: *fMRI: adaptive signal detection (top) and segmentation (bottom)*

The first research theme in statistical and machine learning is that of novelty (or outlier) detection. A central and fruitful focus is the linking of this problem to the theory of classification on the one hand, and of multiple tests (thus linking it to the previous area) on the other. The second research theme concerns the study of iterative and nonlinear estimation methods, such as partial least squares, in the framework of statistical learning in a kernel space. This family of methods is very efficient in practice for a large number of applications, but not yet fully understood. In particular, a crucial point is the choice of the optimal stopping time. Finally, a third research direction currently in development concerns the automated selection and combination of heterogeneous hand-coded features in a collaborative environment. This is the focus of the EU-funded project MASH (Massive Sets of Heuristics), where WIAS will collaborate with four partners from Switzerland, France, and the Czech Republic.

Functional magnetic resonance imaging (fMRI) is utilized both in neuroscience research as well as in clinical applications, such as diagnosis and treatment of brain lesions, to investigate human brain function on small spatial scales. Inherent problems in the analysis of fMRI data are an accurate modeling of sparse spatio-temporal structures, multiple testing for signal detection, and dimension reduction in the presence of poor signal to noise ratios (SNR).

The analysis of fMRI data requires a substantial use of statistical models and methods. Spatially adaptive smoothing has been shown to overcome essential problems with decreased SNR in high resolution fMRI; see [6]. A newly developed adaptive segmentation approach based on multiscale testing leads to a unified method for adaptive smoothing and signal detection. The collaboration with partners, e.g., from Cornell University and the Bernstein Center for Computational Neuroscience, was continued, and the R-package `fmri` was extended.

Diffusion weighted imaging (DWI) is the main neuroscience tool to investigate fiber structure in tissue. In neuroscience, DWI is used to measure anisotropy of water diffusion, which is believed to correspond to the anatomical structure in the white matter area of the brain. The spatial distribution of strength and main directions of anisotropy is used, e.g., for diagnosis of stroke and surgical planning. Further research interests include fiber tracking and investigation of brain connectivity. The common description of anisotropy is based on the diffusion tensor (DTI) model. Statistical methods developed in the research group for structure enhancement within the diffusion tensor model are now investigated for their diagnostic power on clinical data by our partners at the University of Münster. Research is now focused on models for high angular resolution DWI (HARDI). Such models are suitable to describe subvoxel effects like fiber crossings that can not be addressed by DTI. The R-package `dti` has been extended to include methods for HARDI data.

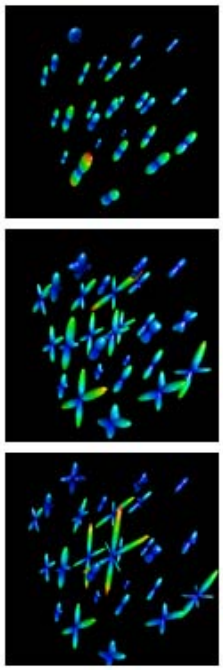

Fig. 2: *Orientation densities from tensor model (top) and tensor mixtures of order 2 (center) and 4 (bottom)*

Applied mathematical finance

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

Highlights 2009:

- Habilitation: John Schoenmakers at Humboldt University of Berlin
- Ph.D.: Stanley Matthew at Technical University of Frankfurt, supervision: John Schoenmakers
- Integration of Peter Friz, new chair holder at TU Berlin, into the research group
- Monograph: *Multidimensional Stochastic Processes as Rough Paths. Theory and Applications* by Peter Friz and Nicolas Victoir

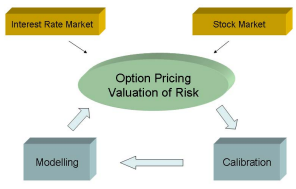

Fig. 3: *Interplay between modeling, pricing, calibration, and data*

In finance there is an increasing demand for effective solutions to optimal control problems for real-world typically high-dimensional financial problems. In [4], several regression based Monte Carlo algorithms for solving multi-dimensional stochastic control problems were developed and rigorously analyzed. The methods in [4] are adapted for tackling problems occurring in portfolio optimization under transaction costs and portfolio liquidation.

The cubature method of Kusuoka, Lyons, and Victoir constitutes a new technology, inspired by rough path theory, that allows to accelerate classical Monte Carlo methods by orders of magnitude; its weak convergence on path space (for instance, applicable to barrier options) remained an open problem conjectured in the literature. It turns out that a suitably flexible (rough path) version of Donsker's invariance principle is precisely the key to this question [1].

Financial modeling with affine processes became very popular in the recent literature due to their rich dynamics and realistic implied volatility patterns. New efficient methods for computing the

characteristic function of general affine processes are developed in a ground-breaking article [3]. There, functional series expansions are derived for classes of holomorphic transforms of the state space vector, which are holomorphic in some neighborhood of time zero and the positive real line. In particular, in the context of option pricing, these expansions allow for computing the characteristic function of general affine price processes in the presence of jumps. Extensions to more general transforms and more general processes are currently in progress.

The general principle of relating the shape of implied volatility to moment explosion [2] becomes fully computable in affine models. In fact, the known refined volatility expansions of Gulishashvili and Stein, currently restricted to the zero-correlation case, appear to be tractable in the general case using affine methods.

In the area of pricing and hedging high-dimensional Bermudan options, a nonparametric regression method was studied in [5], where optimal rates of convergence were derived and the choice of the number of Monte Carlo trajectories was considered.

In electricity markets, the evaluation of (swing) options requires efficient algorithms for multiple stopping problems. For standard American options, hence the standard stopping problem, algorithms based on the dual martingale representation are very popular. For multiple exercise options, hence the multiple stopping problem, there exist dual representations that require a set of (approximative) martingales *and* a set of (approximative) stopping times. A (pure) dual representation in terms of martingales only was, however, not known before. This representation is currently developed and it is shown that it allows for more natural and efficient algorithms.

Many problems in risk management require optimization methods for advanced risk measures and utility functionals rather than optimization of the ordinary expectation and minimization of the standard Value at Risk. In this context, new representation methods are developed that allow for a numerical treatment of such problems. These methods include dual methods and methods based on policy iteration for nonlinear expectations. As such they may be seen as one of the first approaches to tackle general risk measures numerically.

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

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

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

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

The complexity of the problems treated arises from various strong couplings, for example, interface motion producing mechanical stresses, changing electromagnetic fields influencing flow patterns, chemical reactions, the appearance of precipitates in crystals and the formation of quantum dots on crystalline surfaces leading to lattice deformations, nonlocal radiation fields interacting with nonconvective heat conduction, and long-range interatomic interactions leading to nonlocal PDEs.

Highlights

1. The paper "Optimal control of 3D state-constrained induction heating problems" by Pierre-Étienne Druet et al., see [1], describes a theoretical breakthrough within the project C9 "Numerical simulation and control of sublimation growth of semiconductor bulk single crystals" of the DFG Research Center MATHEON. The heating coils of a crystal growth device can now be directly controlled by Maxwell's equations. Moreover, the auxiliary assumptions (Fredholm alternative) to treat the heat radiation problem can now be avoided.

2. The German Patent and Trade Mark Office granted the patent DE 10 2009 028 548 on "Device and Method for Producing Crystals from Electro-conducting Melt". The subject of the patent was studied within the context of the interdisciplinary project KRIST$\widetilde{MAG}$®, which was completed in July 2008. Olaf Klein from RG 7 is among the inventors with 20 %.

Furthermore, Olaf Klein participates with 10 % in a new patent application, DE 10 2009 027 436.7, which is also based on the KRIST$\widetilde{MAG}$® technology. For the first time, a crystal of rectangular shape could be grown within a growth device of cylindrical symmetry.

3. A new model for phase segregation due to Paolo Podio-Guidugli (Rome) was studied. The model, which is based on Gurtin's balance of contact and distance microforces, leads to a new class of

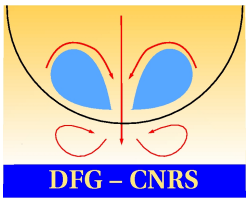
nonlinearly coupled differential equations, namely

– the balance of microforces $$\kappa\,\rho_t - \Delta\rho + f'(\rho) = \mu\,, \qquad (1)$$

– and the energy balance $$(-\mu^2\,\rho)_t = \mu(\kappa\,\rho_t^2 + \bar{\sigma})\,. \qquad (2)$$

Here, ρ is an order parameter, μ is the chemical potential, $\kappa > 0$ the mobility coefficient, and $\bar{\sigma}$ a given function. The coarse-grain free energy f is typically of the form $f = f_1 + f_2$, where f_2 is smooth and $f_1(\rho) = \rho\ln(\rho) + (1-\rho)\ln(1-\rho)$. In [2], existence, uniqueness, and asymptotic behavior as $t \to +\infty$ of a weak solution to an initial-boundary value problem for the system (1) and (2) was proved.

4. Wolfgang Dreyer, jointly with Christiane Kraus from the Leibniz Group *Modeling of Damage Processes*, successfully applied for a three-year funding for the subproject A3 "Modeling and sharp interface limits of local and nonlocal generalized Navier–Stokes–Korteweg systems" within the interdisciplinary framework of the DFG-CNRS Research Unit 563 "Micro-Macro Modelling and Simulation of Liquid-Vapor Flows". In particular, the heat conduction problem is coupled to generalized Navier–Stokes–Korteweg models in this project. The experimental validation of various benchmark tests is carried out at the University of Göttingen.



5. Barbara Wagner contributed to the successful proposal "PVcomB – Competence Centre Thin-Film- and Nanotechnology for Photovoltaics Berlin". The centre is jointly operated by the Helmholtz Centre Berlin for Materials and Energy and the DFG Research Center MATHEON.

6. Within the newly established DFG Priority Program SPP 1506 "Transport Processes at Fluidic Interface", Barbara Wagner and Dirk Peschka, jointly with Ralf Seemann (Max Planck Institute for Dynamics and Self-organization, Göttingen, and University of Saarbrücken), were succesful with their interdisciplinary postdoc proposal on "Mathematical modeling, analysis, numerical simulation of thin liquid bilayers and validation experiments".

Funded projects with industrial collaboration

In the past years, the research group has acquired large competence in the mathematical modeling, analysis, and simulation of technical processes in the context of the production of new materials. The following three examples may give some illustration.

1. The interdisciplinary project AVANT*SOLAR* is financed by industrial partners and the "Zukunftsfonds" of the Federal State of Berlin. The increasing demand for solar silicon requires the design of a new generation of crystal growth devices. The research group contributes with simulations (i) of the global temperature field inside the growth device, (ii) the transport of unwanted substances in the melt in front of the liquid–crystal interface, and (iii) its geometrical shape, in particular, at the triple line where crystal, melt, and chamber wall converge. For example, the WIAS team has to solve the initial and boundary value problem for Navier–Stokes equations coupled to a reaction-diffusion system in an applied time-dependent magnet field. A challenge within this subproject is the incorporation of data concerning the magnetic field that result from a different numerical grid than the one that is used to solve the Navier–Stokes equations. This fact constitutes a non-

trivial problem. For more details see the Scientific Highlights article "Mathematical Modeling and Analysis in the Context of Crystal Growth Phenomena" on page 18.

2. In collaboration with Andreas Münch from the University of Oxford, the work on an industrial-funded project to design a software package of a multi-wall device for surface coating, financed until April 2010, was continued. The software consists of four components: (i) flow simulation with a free liquid–air interface, (ii) elastomer simulation with a solid–liquid interface, (iii) coupling of both phenomena, and (iv) linear stability analysis.

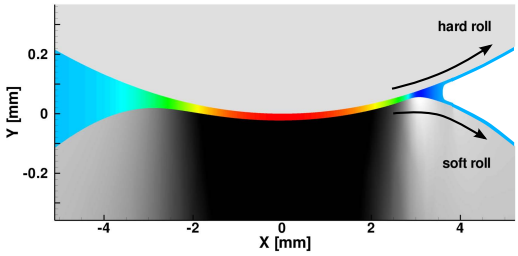


Fig. 1: *Coating process of a Newtonian liquid onto a hard and an elastic roll. The rainbow colors indicate pressure distribution in the liquid, and the gray-scale colors pressure in the elastic body*

Here, the contact problem between an elastomer substrate and a liquid film constitutes a multi-scale problem because the domain ratio *height/width* is of order 10^{-4}, yielding many elements in the spatial discretization and a rather long runtime in the classical treatment of the Navier–Stokes equations. For this reason, in some parts of the domain the lubrication approximation is applied, resulting in a runtime reduction up to a factor 50 with a loss of accuracy below 0.1 %.

3. In collaboration with Eberhard Bänsch (University of Erlangen), the computational fluid dynamics (CFD) software NAVIER was extended to describe the dynamics of toner particles within an ionized liquid. The industrial-funded project concerns the coupling of particle dynamics to hydrodynamics, drift-diffusion equations, and electrostatics.

Funded under Priority Programs of the German Research Foundation

The work on the problem "Mathematical modeling, analysis, numerical simulation of thin films and droplets on rigid an viscoelastic substrates, emphasizing the role of slippage" within the DFG Priority Program SPP 1164 "Nano- and Microfluidics: Bridging the Gap between Molecular Motion and Continuum Flow" was continued. Relying on the Navier–Stokes equations, a lubrication model, and a finite-difference code, the crucial parameters that control the quasi-stationary profile of a gliding droplet due to gravitation were identified. Among them are the surface tension, inclination, and sliding properties of the substrate. With increasing gravitational force, deviations of droplet profiles and velocity fields according to Navier–Stokes (respectively, the lubrication model) could be observed. For a continuation of the studies a proposal within the new DFG Priority Program SPP 1506 "Transport Processes at Fluidic Interfaces" was written.

Selected MATHEON projects

1. The project group C10 “Modelling, asymptotic analysis and numerical simulation of the dynamics of thin film nanostructures on crystal surfaces” of the DFG Research Center MATHEON, in collaboration with Andreas Münch, University of Oxford, continued the study of self-assembly of quantum dots on crystalline substrates. In [3] a consistent reduction of a continuum model that relies on small slopes of surfaces was carried out. For anisotropic surfaces and a stochastic disturbed atomic flux this leads to a single PDE, taking into account the elastic energy that is induced by the misfit between film and substrate and surface energy that controls the separation of the individual quantum dots. Application of pseudo-spectral methods allows for simulations in large domains without runtime problems.

2. In collaboration with members of the University of Oxford, the MATHEON project group C26 “Storage of hydrogen in hydrides” developed a new model for generic storage problems where the storage system consists of a large number of storage particles. Among these problems are the storage of hydrogen in magnesium particles, the storage of lithium in iron-phosphate particles forming the cathode of lithium-ion batteries, and balloons that may serve to store air. The central object of the model is a probability density describing the evolution of the filling of the ensemble of storage particles. It is calculated by an initial and boundary value problem for a new nonlocal and nonlinear PDE of Fokker–Planck type.

Fig. 2: *Interconnected balloons exhibit two coexisting phases consisting of balloons with large (respectively, small) filling*

The model gives a natural explanation of the observed phase transition and hysteresis of many-particle storage systems. In the context of the improvement of lithium ion-batteries, the model solves an outstandingly important problem. More details concerning the equilibria of storage problems are to be found in [4].

Ph.D. students

Wolfgang Dreyer, Jürgen Sprekels, and Barbara Wagner, jointly with other partners, guide and supervise 14 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, and in collaboration with the Technical University (TU) and the Humboldt University (HU) of Berlin, the University of Basel, and the University of Stuttgart.

In 2009, five Ph.D. theses were successfully completed.

- Analysis of a coupled system of partial differential equations modeling the interaction between melt flow, global heat transfer, and applied magnetic fields in crystal growth: The topic is part of MATHEON project C9. Moreover, it is related to the interdisciplinary project KRISTMAG®, where two industrial companies, physicists, engineers, and mathematicians have designed new heater-magnet modules to control the melt flow and the shape of the melt/crystal interface during crystal growth. Pierre-Étienne Druet was awarded his doctorate with “highest distinction” (summa cum laude) from HU Berlin.
- Macroscopic diffusion models for precipitation in crystalline gallium arsenide: The models concern coupled systems of diffusion equations with mechanical interactions and their mean-field

limits to describe the evolution of unwanted liquid droplets in a crystal. The topic is studied in an industrial collaboration and is part of the MATHEON project C14. Sven-Joachim Kimmerle passed his Ph.D. examination at HU Berlin with "high distinction" (magna cum laude).

– Derivation, analysis, and numerics of reduced ODE models describing coarsening dynamics of liquid droplets: The study is based on thin-film lubrication models and concerns their reduction to simpler models that describe late-phase dynamics of pattern formations of droplets on substrates. Georgy Kitavtsev was a member of the DFG Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", and he passed his Ph.D. examination at HU Berlin with "high distinction" (magna cum laude). For more details see the Scientific Highlights article "Dewetting of Complex Liquids" in the Annual Research Report 2008.

– Solvability of pseudo-monotone/monotone systems and application to a model of phase transitions: A "notorious" complex system of phase field equations with mechanical coupling, which is relevant to describe the behavior of micro-solders, is reformulated into a general system of evolution equations so that the theory of pseudo-monotone/monotone operators can be applied. Donat Wegner was also a member of the DFG Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", and he passed his Ph.D. examination at HU Berlin also with "high distinction" (magna cum laude).

– Mathematical modeling and experimental study of the growth kinetic and spatial organization of chondrocytes during monolayer culture: Viviana Palumberi passed her Ph.D. examination at the University of Basel. The topic belongs to the field of biomathematics and tissue engineering. The model that was developed and studied combines time-lag (delay) with logistic equations. The latter are used to characterize spatio-angular cell–cell interaction coupled with logistic growth.

Miscellaneous

Barbara Wagner is Deputy Chairperson of the Council of the DFG Research Center MATHEON, and in 2009 she became a member of the SIAM Selection Committee for the *Julian Cole Lectureship*. Furthermore, Barbara Wagner was awarded an *OCCAM Visiting Fellowship*.

References

[1] P.-É. DRUET, O. KLEIN, J. SPREKELS, F. TRÖLTZSCH, I. YOUSEPT, *Optimal control of 3D state-constrained induction heating problems with nonlocal radiation effects*, WIAS Preprint no. 1422, 2009, submitted.

[2] P. COLLI, G. GILARDI, P. PODIO-GUIDUGLI, J. SPREKELS, *Global solution and long-time behavior for a problem of phase segregation of the Allen–Cahn type*, to appear in: Math. Models Methods Appl. Sci.

[3] M.D. KORZEC, P.L. EVANS, *From bell shapes to pyramids: A continuum model for self-assembled quantum dot growth*, WIAS Preprint no. 1434, 2009, submitted.

[4] W. DREYER, C. GUHLKE, R. HUTH, *The behavior of a many particle cathode in a lithium-ion battery*, WIAS Preprint no. 1423, 2009, submitted.

3.8 Leibniz Group 1 "Coupled Flow Processes in Energy and Environmental Research"

Efficient and accurate simulation of coupled flow processes is an important and in many cases not yet satisfactorily solved problem in many applications in fields like energy, climate, geological, and environmental research. The Leibniz group was established in the framework of the competition procedure of the Leibniz Association, as a part of a research network joining WIAS, the Free University of Berlin, the Potsdam Institute for Climate Impact Research, and the University of Erlangen. It focuses on coupled flow processes in electrochemical systems like fuel cells and the coupling between flow processes in the atmosphere and the soil. The Leibniz group closely cooperates with the Research Group *Numerical Analysis and Scientific Computing* (RG 3).

One focus of the group at WIAS is the mass conservative coupling of incompressible fluid flow and species transport. Provided that the discrete velocity field is divergence-free in the discrete sense, a method guaranteeing physically relevant bounds of species concentrations in transport equations (discrete maximum principle) is the Voronoi box based finite volume method on boundary-conforming Delaunay meshes, which is developed in RG 3. For velocity approximations resulting from divergence-free finite elements like the Scott–Vogelius element, this condition can be satisfied. See [2] for a case where this property is important for the approximation of fluid flow itself. The resulting combined finite element / finite volume ansatz has been successfully applied in the numerical modeling of electrochemical flow cells [1].

Current work at WIAS focuses on the development of finite volume methods for incompressible fluid flow that result in discretely divergence-free velocity fields.

The problem of coupling models of free flow and porous media flow arises in a number of applications, including fuel cells and redox flow cells with flow-through electrodes. A deeper understanding of the choice of the interface condition aims at the development of a mass-conservative finite volume method, which includes appropriate coupling conditions at the interface. For a more elaborate discussion of this question, see the Highlights article on page 49.

The main application field of the group is electrochemistry. Current investigations focus on electrochemical flow cells, being useful tools for the experimental investigation of electrocatalytic processes. The models developed by the group support experimental work by investigating hypotheses on the structure of catalytic reaction networks.

References

[1] J. Fuhrmann, A. Linke, H. Langmach, H. Baltruschat, *Numerical calculation of the limiting current for a cylindrical thin layer flow cell*, Electrochimica Acta, **55** (2009), pp. 430–438.

[2] A. Linke, *Collision in a cross-shaped domain — A steady 2D Navier–Stokes example demonstrating the importance of mass conservation in CFD*, Comput. Methods Appl. Mech. Engrg., **198** (2009), pp. 3278–3286.

3.9 Leibniz Group 2 "Modeling of Damage Processes"

In the framework of the competition "Pakt für Forschung und Innovation" of the Leibniz Association, Dorothee Knees and Christiane Kraus successfully applied for the funding of a research group at WIAS. This grant provides the basis for the new Leibniz Group 2 that was formed at WIAS in 2009, working on the modeling, analysis, and simulation of damage processes.

In many materials, the failure of the entire device is the result of damage processes on a very small scale. Microvoids and microcracks emerge due to stresses. Under further loading, these voids and cracks grow, coalesce, and finally lead to the failure of the whole device by developing a macroscopic crack. For a realistic description of the whole damage behavior, the processes on all scales should be modeled in detail. However, such models are much too complex to serve as a basis for numerical simulations. Therefore, the aim of the Leibniz Group is to construct and analyze effective, macroscopic damage and fracture models where the interplay between the different scales is justified in a mathematically rigorous way.

The group works on the analytical and numerical modeling of *phase separation* and *damage processes* in alloys with the intention to predict and finally optimize the strength and lifetime of solder joints. For this purpose, phase-field models of Cahn–Hilliard type are investigated that may include elastic effects, anisotropy, or damage. Adaptive finite element methods were developed, and a posteriori error estimates, which are robust for vanishing interface width, were derived. In addition, rigorous results for sharp interface limits of phase field energies, including spatially inhomogeneous anisotropic interfacial energy and elasticity, were attained.

Fig. 1: *Coarsening of a binary alloy: Anisotropic elasticity tensor leads to alignment of phase boundaries (Rüdiger Müller (Leibniz Group 2) and Sören Bartels (University of Bonn))*

Starting from the experience gained from regularity theory and homogenization in elasto-plasticity, current research also focuses on the derivation of an effective damage model based on microcrack evolution of Griffith type. For an overview of regularity properties in elasto-plasticity, we refer to the Scientific Highlights article by Dorothee Knees on page 44.

The research group participates in the renewal proposal of the DFG Research Center MATHEON for the period 2010–2014 with a project on damage evolution in solder alloys.

Christiane Kraus and Wolfgang Dreyer (Research Group 7) successfully applied for a three-year funding of a Ph.D. position within the DFG-CNRS Research Unit 563 "Micro-Macro Modelling and Simulation of Liquid-Vapour Flows".

Fig. 2: *Research Unit 563 (supported by DFG and CNRS)*

Finally, Dorothee Knees and Sergiy Nesenenko (TU Darmstadt) organized a Young Researchers' Minisymposium at the Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM) 2009 in Gdańsk where analytical and numerical aspects of elasto-plastic models were discussed.

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, Undergraduate-degree Supervision

A.1.1 Calls

1. G. Blanchard, Junior professorship, October 1, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II.
2. ———, W3 professorship, November 27, Universität Potsdam, Mathematisch-Naturwissenschaftliche Fakultät.
3. W. Dreyer, W3 professorship, June 8, Technische Universität Berlin, Fakultät V — Verkehrs- und Maschinensysteme, Honorary Professorship.
4. M. Ehrhardt, W2 professorship, July 3, Bergische Universität Wuppertal, Fachbereich Mathematik und Naturwissenschaften.
5. A. Rohde, Junior professorship, April 28, Universität Hamburg, Fakultät für Mathematik, Informatik und Naturwissenschaften.

A.1.2 Awards and Distinctions

1. G. Kitavtsev, *Best Presentation at the European Postgraduate Fluid Dynamics Conference 2009*, July 16.
2. D. Knees, *Robert Bosch Stiftung: Fast Track Scholarship*, 2008–2010.
3. A. Mielke, *Coordinator of the Theoretical Mechanics Group of the Centro di Ricerca Matematica "Ennio De Giorgi", Pisa, Italy*.
4. ———, *Member of the Council of the International Society for Interaction of Mathematics and Mechanics (ISIMM)*.
5. J. Sprekels, *Chairman of the Board of Forschungsverbund Berlin e.V.*
6. ———, *Coordinator of the International Mathematical Science Institutes (IMSI)*.

A.1.3 Habilitations

1. U. Bandelow, *Advanced mathematical modeling of nonlinear optoelectronic and photonic components*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, July 15.
2. J.G.M. Schoenmakers, *Robust LIBOR modelling and pricing of derivative products*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, July 6.

A.1.4 Ph.D. Theses

1. E. Diederichs, *Non-Gaussian component analysis with applications to biomolecular confirmations*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisors: Prof. Dr. Ch. Schütte, Prof. Dr. V. Spokoiny, July 31.

2. E. Giacomini, *Time varying adaptive copulae and dynamic semiparametric factor models with applications in finance*, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, supervisor: Prof. Dr. V. Spokoiny, January 30.
3. S.-J. Kimmerle, *Macroscopic diffusion models for precipitation in crystalline gallium arsenide*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisors: Prof. Dr. B. Niethammer, Prof. Dr. W. Dreyer, September 21.
4. S.S. Mathew, *Multicurrency extension of a multiple stochastic volatility LIBOR market model*, Goethe-Universität Frankfurt am Main, Fachbereich Mathematik und Informatik, supervisor: Dr. J.G.M. Schoenmakers, January 20.
5. V. Palumberi, *Chondrocyte growth dynamics and spatial pattern formation*, Universität Basel, Philosophisch-Naturwissenschaftliche Fakultät, supervisors: Prof. Dr. M. Grote, Priv.-Doz. Dr. B. Wagner, April 16.
6. A. Pimenov, *Stability and bifurcations of systems with hysteresis and multistable systems*, National University of Ireland, Department of Applied Mathematics, Cork, supervisors: Dr. D.I. Rachinskii, Priv.-Doz. Dr. A.G. Vladimirov, September 28.
7. D. Wegner, *Solvability of pseudomonotone-strongly monotone systems and application to a model of phase transitions*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisors: Prof. Dr. J. Sprekels, Prof. Dr. W. Dreyer, November 12.
8. P.-É. Druet, *Analysis of a coupled system of partial differential equations modeling the interaction between melt flow, global heat transfer and applied magnetic fields in crystal growth*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. J. Sprekels, February 5.
9. J. Ehrt, *Cascades of heteroclinic connections in hyperbolic balance laws*, Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. B. Fiedler, November 17.
10. G. Kitavtsev, *Derivation, analysis and numerics of reduced ODE models describing coarsening dynamics of liquid droplets*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisors: Prof. Dr. B. Niethammer, Priv.-Doz. Dr. B. Wagner, November 10.
11. A. Weiss, *Aspects of microscopic modelling in finance*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. A. Bovier, October 16.

A.1.5 Undergraduate-degree Supervision

1. O. Akdogan, *Monte Carlo evaluation of callable products in jump-diffusion models* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Dr. J.G.M. Schoenmakers, May 27.
2. E. Dremkova, *A high-order compact method for nonlinear Black–Scholes option pricing equations with transaction costs* (master thesis), Halmstad University, Sweden, Master's Programme in Financial Mathematics, supervisor: Priv.-Doz. Dr. M. Ehrhardt, June 1.
3. V. Egorova, *High-order compact methods for the American option pricing problem* (master thesis), Halmstad University, Sweden, Master's Programme in Financial Mathematics, supervisor: Priv.-Doz. Dr. M. Ehrhardt, June 1.
4. H. Hanke, *Homogenisierung in der Gradientenplastizität* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. A. Mielke, January 21.
5. Ch. Heinemann, *Homogenisierung von nichtlinearen Schrödingergleichungen* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. A. Mielke, July 27.

6. A. Ivanova, *High-order compact methods for the American option pricing problem* (master thesis), Halmstad University, Sweden, Master's Programme in Financial Mathematics, supervisor: Priv.-Doz. Dr. M. Ehrhardt, June 1.
7. D. Klindworth, *Discrete transparent boundary conditions for multiband effective mass approximations* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Priv.-Doz. Dr. M. Ehrhardt, September 16.
8. A. Mezentsev, *Valuation of installment options* (master thesis), Halmstad University, Sweden, Master's Programme in Financial Mathematics, supervisor: Priv.-Doz. Dr. M. Ehrhardt, June 1.
9. A. Pomelnikov, *Valuation of installment options* (master thesis), Halmstad University, Sweden, Master's Programme in Financial Mathematics, supervisor: Priv.-Doz. Dr. M. Ehrhardt, June 1.
10. O. Vassilieva, *A new method of pricing multi-options using Mellin transforms and integral equations* (master thesis), Halmstad University, Sweden, Master's Programme in Financial Mathematics, supervisor: Priv.-Doz. Dr. M. Ehrhardt, June 1.

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)

"Biotechnologie, Pharmazie und Chemie: Verbundprojekt SimPaTurS: Gekoppelte Simulation von Partikelpopulationen in turbulenten Strömungen" (Biotechnology, Pharmacy and Chemistry: Joint Project SimPaTurS: Coupled Simulation of Particle Populations in Turbulent Flows); subproject "Turbulente Strömungen" (Turbulent flows; in RG 3)

Bundesministerium für Wirtschaft und Technologie (Federal Ministry of Economics and Technology), Berlin

– **Zentrales Innovationsprogramm Mittelstand (ZIM): Kooperationen (Central Innovation Program for SMEs: Cooperations)**

Cooperative Project "Neue Messmethodik für die Werkstoffentwicklung" (New methods of measurements for the development of materials), subproject "Modellierung, Simulation und Parameteridentifikation" (Modeling, simulation and parameter identification; 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)

B20: "Optimization of gas transport" (in RG 4)

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)

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

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

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

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

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

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

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

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

– Collaborative Research Center (SFB) 555, Humboldt-Universität zu Berlin, “Komplexe Nichtlineare Prozesse” (Complex Nonlinear Processes)

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

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

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

  B7: “Calibration and pricing errors in risk management” (in RG 6)

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

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

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

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

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

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

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

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

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

– Priority Program SPP 1276: “MetStröm: Skalenübergreifende Modellierung in der Strömungsmechanik und Meteorologie” (MetStröm: Multiple Scales in Fluid Mechanics and Meteorology)

  „Referenzexperimente im mehrphasigen Windkanal, numerische Simulationen und Validierung“ (Reference experiments in a multiphase wind tunnel, numerical simulations and validation; in RG 3)

– Research Unit FOR 718 “Analysis and Stochastics in Complex Physical Systems”, Berlin and Leipzig

  “Systems with many degrees of freedom: Probabilistic and constructive field theory methods” (in RG 5)

  Coordinator Program: W. König (Head of RG 5)

– 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)**

“Direkte und inverse Streuprobleme bei elastischen Wellen” (Direct and inverse scattering problems for elastic waves; in RG 4)

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

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

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

Leibniz-Gemeinschaft (Leibniz Association), Bonn and Berlin

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

“Gekoppelte Strömungsprozesse in Energie- und Umweltforschung” (Coupled flow processes in energy and environmental research, coordinator: J. Fuhrmann, LG 1)

“Modellierung von Schädigungsprozessen” (Modeling of damage processes; in LG 2)

Deutscher Akademischer Austauschdienst (German Academic Exchange Service), Bonn

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

– 1 scholarship holder (in RG 6)

Technologiestiftung Berlin (Technology Foundation Berlin)

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

International Projects

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

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

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

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

– 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” (in RG 5)

Mission-oriented research (examples)

- ALSTOM (Switzerland) Ltd., Baden: “Prozesssimulation bei industriellen Gasturbinen” (Process simulation for industrial gas turbines; in RG 3 and RG 6)
- Electricité de France (EDF), Clamart: “Optimization problems with chance constraints applied to electricity portfolio” (in RG 4)
- European XFEL GmbH, Hamburg: “Numerical investigation of the movement of large clouds in depleted Si detectors” (in RG 3)
- Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin: “Mathematische Modellierung und Simulation von MOPA-Diodenlasern” (Mathematical modeling and simulation of MOPA diode lasers; in RG 2)
- Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin: “Wellenlängenstabilisierte Halbleiterlaser” (Wavelength-stabilized semiconductor lasers; in RG 2)
- Ferdinand-Braun-Institut für Höchstfrequenztechnik, Berlin: “Ausbreitung von Lichtimpulsen in trapezförmigen Halbleiterlaserverstärkern” (Propagation of optical pulses in trapezoidal semiconductor amplifiers, subproject in BMBF joint project “Erforschung und Entwicklung von innovativen hybrid-integrierten Diodenlaser-Komponenten und Systemen” (InDiLas — Investigation and Development of Innovative Hybrid Integrated Diode Laser Components and Systems; in RG 2)
- Fraunhofer-Institut für Integrierte Schaltungen, Entwurfsautomatisierung (EAS), Dresden: “Entwicklung einer Simulationsplattform” (Development of a simulation platform; in RG 3)
- HSH Nordbank AG, Kiel: “Robuste Kalibrierung des erweiterten Libor-Markt-Modells”(Robust calibration of the expanded Libor market model, in RG 6)
- International Intellectual Group, Inc., Staten Island: “A conical diffraction solver for multiple penetrating profiles” (in RG 4)
- Landesbank Berlin AG: “Entwicklung erweiterter Libor-Markt-Modelle, Kalibrierung, Bewertung und Replikation komplex strukturierter Produkte” (Development of expanded Libor market models, calibration, pricing, and replication of complex structured products, in RG 6)
- Physikalisch-Technische Bundesanstalt, Braunschweig and Berlin: “Vermessung von Lithographiemasken durch Scatterometrie” (Measurements of lithographic masks based on scatterometry; in RG 4)
- Rücker EKS GmbH, Weingarten: “Simulations- und Optimierungsaufgaben bei der Fabrikplanung und virtuellen Inbetriebnahme” (Simulation and optimal control tasks in production planning and virtual commissioning; in RG 4)
- Zuse Institute Berlin: “Entwicklung von Verfahren zur Optimierung von Gastransportnetzen” (Development of methods for the optimization of gas networks, sub-order for E.ON Gastransport GmbH Essen, in RG 4)

A.3 Membership in Editorial Boards[2]

1. P. Friz, Editorial Board, Annals of Applied Probability, Institute of Mathematical Statistics (IMS), Beachwood, Ohio, USA.
2. M. Ehrhardt, Editorial Board, Advances in Applied Mathematics and Mechanics, Global Science Press, Wanchai, Hong Kong.
3. ———, Editorial Board, International Journal of Computer Mathematics, Section B: Computational Methods: Applications, Taylor & Francis, Abingdon, UK.
4. ———, Editorial Board, Numerical Mathematics: Theory, Methods and Applications, Global Science Press, Nanjing, China.
5. R. Henrion, Editorial Board, International Journal of Management Science and Engineering Management (MSEM), World Academic Press, Liverpool, UK.
6. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
7. ———, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Dordrecht, The Netherlands.
8. W. König, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
9. V. Krätschmer, Advisory Board, Applied Computational Intelligence and Soft Computing, Hindawi Publishing Corporation, New York, USA.
10. P. Krejčí, Editor-in-Chief, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.
11. P. Mathé, Editorial Board, Journal of Complexity, Elsevier, Amsterdam, The Netherlands.
12. ———, Editorial Board, Monte Carlo Methods and Applications, Walter De Gruyter, Berlin, New York, USA.
13. A. Mielke, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
14. ———, Editor-in-Chief, Journal of Nonlinear Science, Springer Science+Business Media, New York, USA.
15. ———, Editor-in-Chief, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
16. ———, Co-Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
17. ———, Editorial Board, Archive for Rational Mechanics and Analysis, Springer-Verlag, Berlin, Heidelberg.
18. ———, Editorial Board, European Series in Applied and Industrial Mathematics: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
19. ———, Editorial Board, Mathematical Models and Methods in Applied Sciences, Imperial College Press, London, UK.
20. H. Neidhardt, Editorial Board, Advances in Mathematical Physics, Hindawi Publishing Corporation, New York, USA.
21. J. Polzehl, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.
22. ———, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, The Netherlands.
23. J. Sprekels, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.

[2] Memberships in editorial boards by guests during their long-term stay at WIAS have been listed in front of those by the collaborators of WIAS.

24. ———, Editorial Board, Mathematics and its Applications, Annals of the Academy of Romanian Scientists, Academy of Romanian Scientists, Bucharest, Romania.
25. ———, Editor, Advances in Mathematical Sciences and Applications, Gakkōtosho, Tokyo, Japan.
26. W. Wagner, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.

A.4 Conferences, Colloquia, and Workshops

Workshop "Nonlinear Optics in Guided Geometries"
Berlin, May 18–20
Organized by: WIAS (RG 2), Max Born Institute (MBI) for Nonlinear Optics and Short Pulse Spectroscopy, Matheon Project Group D14 "Nonlocal and nonlinear effects in fiber optics"
Supported by: DFG Research Center Matheon, WIAS

The workshop aimed at bringing together experts working on the generation, propagation, compression, and broadening of short optical pulses. The workshop was attended by 49 participants from 10 countries and included 25 invited and 9 contributed talks.

The major topics were:

(1) ultrashort and few-cycle optical pulses
(2) femtosecond filamentation
(3) pulse self-compression
(4) solitons in photonic crystal media
(5) optical dissipative solitons

Researchers with different backgrounds, i.e., theoreticians and experimentalists working on mathematical and physical problems as well as on technological applications were invited. The interdisciplinary approach and careful scheduling allowed for intense discussions and were highly acknowledged by the participants.

5th Colloquium of the DFG 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)
Berlin, June 23
Organized by: WIAS (RG 4), DFG (SPP 1204)
Supported by: DFG (SPP 1204)

The goal of this workshop was to bring together the groups participating in the DFG Priority Program SPP 1204. The 24 participants discussed issues related to the simulation and control of multi-phase steels, various aspects of hot and cold rolling, as well as process chain models for sheet metal forming and hammer forging.

Workshop "Coupled Models in Energy, Hydrology and Climate Research"
Berlin, October 8–9
Organized by: WIAS (LG 1), Freie Universität Berlin
Supported by: Ruprecht-Karls-Universität Heidelberg, Westfälische Wilhelms-Universität Münster, Freie Universität Berlin, WIAS

The workshop was jointly organized by the Research Network "Coupled Flow Processes in Energy and Environmental Research", funded by the Leibniz Association and coordinated by WIAS (LG 1), and the Network "Adaptive Hydrological Modeling with Applications in Water Management — AdaptHydroMod" funded by the Federal Ministry of Education and Research.

It focused on issues of modeling and simulation of coupled flow processes. Prominent topics were the coupling between free and porous media flow with applications in electrochemistry and hydrology, and between subsurface and surface flow. The workshop had 45 participants from six countries, among them several of the top-level scientists in the field. On this basis, it was possible to develop a number of new and important contacts to scientific groups that can contribute to the improvement of mathematical and numerical models developed in the institute.

Workshop "Structure Adapting Methods"
Berlin, November 6–8
Organized by: WIAS (RG 6), DFG (SFB 649 "Economic Risk"), Center for Applied Statistics and Economics (C.A.S.E., Humboldt University of Berlin)
Supported by: DFG (SFB 649)

The workshop aimed at bringing together experts working on challenging problems in data analysis: high dimensional data (large p, small n), complexity/dimensionality reduction, and adaptation. Researchers with different backgrounds in statistics were invited.

The event was attended by 45 participants from 10 countries and included 14 invited and 8 contributed talks.

The major topics were:

(1) adaptive methods
(2) high-dimensional data
(3) sparse estimation
(4) variable and model selection

Mini-symposium "Nonlinear Dynamics in Quantum Dot Devices"
Berlin, November 9
Organized by: WIAS (RG 2)
Supported by: DFG (SFB 787 "Semiconductor Nanophotonics: Materials, Models, Devices")

Quantum dot lasers demonstrate a number of important advantages as compared to standard quantum well devices with respect to their applications in telecommunications technologies. However, tailoring the characteristics of quantum dot lasers for specific applications is a challenging issue that requires the development of new mathematical models and their analysis. This is hardly achievable without combining the efforts of experimentalists, theoreticians, and specialists in mathematical modeling.

The goal of the mini-symposium organized by Andrei Vladimirov and Matthias Wolfrum was to bring together researchers of several groups from Berlin, Cork, and Brussels, working in the field of experimental investigation and mathematical modeling of operation regimes in quantum dot lasers. The main interest of the participants was focused on mode-locking in quantum dot lasers.

Six invited talks presented at the mini-symposium and the subsequent discussion covered different aspects of the dynamics of quantum dot lasers: experimental study of hybrid mode-locking, injection locking in passively mode-locked lasers, numerical modeling of mode-locked lasers and amplifiers, as well as macroscopic and microscopic modeling of carrier exchange processes in quantum dot materials.

International Conference on Elliptic and Parabolic Equations
Berlin, November 30 – December 4
Organized by: WIAS (RG 1), Matheon Project Group D4 "Quantum mechanical and macroscopic models for optoelectronic devices"
Supported by: DFG Research Center Matheon, WIAS

Elliptic and parabolic PDEs have been powerful models of problems in science and engineering for more than a quarter millennium. The classical solution theory of these equations assumes "perfect" spatial domains and coefficients. However, to deal with real-world problems today, one has to take into account vertices and edges of three-dimensional spatial domains, discontinuous coefficient functions, and various mixed boundary conditions. Suitable regularity for such linear elliptic problems is crucial for the solution theory of corresponding nonlinear elliptic and parabolic equations. This conference examined the progress in this direction, and elliptic and parabolic equations in real space at large. Beyond that scope, one day of the conference was specifically devoted to Navier–Stokes equations.

All in all, 91 renowned scientists participated in the conference. Forty-two extended talks and several short communications and posters were presented.

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

1. U. Bandelow, member of the Program Committee, *9th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD) 2009*, Gwangju Institute of Science and Technology (GIST), Republic of Korea, September 14–18.
2. A. Bianchi, co-organizer, *Summer School in Probability*, Università di Bologna, Italy, July 6–10.
3. J. Fuhrmann, organizer of the invited session "Numerical Modeling in Electrochemistry ", *Conference on Scientific Computing (ALGORITMY 2009)*, Slovak University of Technology, Podbanské, March 15–20.
4. R. Henrion, organizer of the invited session "Chance Constraints", *23rd European Conference on Operational Research (EURO23)*, Bonn, July 5–8.
5. D. Hömberg, co-organizer, Matheon-*SEFI Workshop "Mathematical Education of First-year Engineering Students"*, Technische Universität Berlin, April 6–7.
6. D. Hömberg, organizer of the minisymposium "Mathematical Concepts for the Simulation and Control of Machine Tools", *SIAM Conference on Mathematics for Industry: Challenges and Frontiers (MI09)*, San Francisco, USA, October 9–10.
7. D. Knees, co-organizer of the Young Researchers' Minisymposium "Analytical and Numerical Aspects of Time-dependent Problems with Internal Variables", *80th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2009)*, Gdansk University of Technology, Poland, February 9–13.
8. W. König, organizer, *Berlin-Leipzig Seminar on Analysis and Probability Theory*, Technische Universität Berlin, November 27.
9. A. Mielke, co-organizer, *Workshop on Pulses and Modulations in Nonlinear Systems*, Universität Stuttgart, February 25–27.
10. A. Rathsfeld, member of the Program Committee, *SPIE Europe Optical Metrology 2009*, Munich, June 15–18.
11. A.G. Vladimirov, member of the Technical Program Committee, *Conference on Lasers and Electro-Optics Europe (CLEO/Europe 2009)*, Munich, June 14–19.

A.6 Publications[3]

Monographs (to appear)

[1] P. Friz, N.B. Victoir, *Multidimensional Stochastic Processes as Rough Paths*, vol. 120 of Cambridge Studies in Advanced Mathematics, Cambridge University Press, Cambridge.

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

A.6.1 Editorship of Proceedings and Collected Editions

[1] K. Kunisch, G. Leugering, J. Sprekels, F. Tröltzsch, eds., *Optimal Control of Coupled Systems of Partial Differential Equations*, vol. 158 of Internat. Series Numer. Math., Birkhäuser, Basel et al., 2009, 345 pages.

A.6.2 Outstanding Contributions to Monographs

[1] Q.A. Dang, M. Ehrhardt, G.L. Tran, D. Le, *Chapter 6: On the Numerical Solution of Some Problems of Environmental Pollution, in: Environmental Chemistry Research Progress*, P. Robinson, R. Gallo, eds., Nova Science Publishers, New York, USA, 2009, pp. 199–228.

Contributions to Monographs (to appear)

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

[2] M. Ehrhardt, Ch. Zheng, *Chapter 7: Fast Numerical Methods for the Simulation of Waves in Periodic Structures, in: Wave Propagation in Periodic Media — Analysis, Numerical Techniques and Practical Applications*, M. Ehrhardt, ed., vol. 1 of Progress in Computational Physics (PiCP), Bentham Science Publishers Ltd.

A.6.3 Articles in Refereed Journals

[1] P. Friz, S. Benaim, *Regular variation and smile asymptotics*, Math. Finance, 19 (2009), pp. 1–12.

[2] P. Friz, E. Breuillard, M. Huesmann, *From random walks to rough paths*, Proc. Amer. Math. Soc., 137 (2009), pp. 3487–3496.

[3] P. Friz, M. Caruana, *Partial differential equations driven by rough paths*, J. Differential Equations, 247 (2009), pp. 140–173.

[4] P. Friz, T. Cass, N. Victoir, *Non-degeneracy of Wiener functionals arising from rough differential equations*, Trans. Amer. Math. Soc., 361 (2009), pp. 3359–3371.

[5] P. Friz, H. Oberhauser, *Rough path limits of Wong–Zakai type with modified drift term*, J. Funct. Anal., 256 (2009), pp. 3236–3256.

[6] S. Amiranashvili, U. Bandelow, A. Mielke, *Padé approximant for refractive index and nonlocal envelope equations*, Opt. Commun., 283 (2009), pp. 480–485.

[3] Publications by guests and scholarship holders have been listed in front of those written by the collaborators of WIAS.

[7] D. Belomestny, J. Kampen, J.G.M. Schoenmakers, *Holomorphic transforms with application to affine processes*, J. Funct. Anal., 257 (2009), pp. 1222–1250.

[8] D. Belomestny, Ch. Bender, J.G.M. Schoenmakers, *True upper bounds for Bermudan products via non-nested Monte Carlo*, Math. Finance, 19 (2009), pp. 53–71.

[9] D. Belomestny, S. Mathew, J.G.M. Schoenmakers, *Multiple stochastic volatility extension of the Libor market model and its implementation*, Monte Carlo Methods Appl., 15 (2009), pp. 285–310.

[10] D. Belomestny, G.N. Milstein, V. Spokoiny, *Regression methods in pricing American and Bermudan options using consumption processes*, Quant. Finance, 9 (2009), pp. 315–327.

[11] A. Bianchi, A. Bovier, D. Ioffe, *Sharp asymptotics for metastability in the random field Curie–Weiss model*, Electron. J. Probab., 14 (2009), pp. 1541–1603.

[12] A. Schwaighöfer, T. Schröter, S. Mika, G. Blanchard, *How wrong can we get? A review of machine learning approaches and error bars*, Comb. Chem. High Throughput Screening, 12 (2009), pp. 453–468.

[13] C. Brée, A. Demircan, S. Skupin, L. Bergé, G. Steinmeyer, *Self-pinching of pulsed laser beams during filamentary propagation*, Optics Express, 17 (2009), pp. 16429–16435.

[14] C. Brée, A. Demircan, G. Steinmeyer, *Asymptotic pulse shapes in filamentary propagation of intense femtosecond pulses*, Laser Physics, 19 (2009), pp. 330–335.

[15] P.-É. Druet, *Existence for the stationary MHD equations coupled to heat transfer with nonlocal radiation effects*, Czechoslovak Math. J., 59 (2009), pp. 791–825.

[16] ———, *Existence of weak solution to time-dependent MHD equations coupled to heat transfer with nonlocal radiation boundary conditions*, Nonlinear Anal. Real World Appl., 10 (2009), pp. 2914–2936.

[17] P.-É. Druet, J. Naumann, *On the existence of weak solutions to a stationary one-equation RANS model with unbounded eddy viscosities*, Ann. Univ. Ferrara Sez. VII Sci. Mat., 55 (2009), pp. 67–87.

[18] O. Gloger, M. Ehrhardt, Th. Dietrich, O. Hellwich, K. Graf, E. Nagel, *A threestepped coordinated level set segmentation method for identifying atherosclerotic plaques on MR images*, Comm. Numer. Methods Engrg., 25 (2009), pp. 615–638.

[19] M. Ehrhardt, H. Han, Ch. Zheng, *Numerical simulation of waves in periodic structures*, Commun. Comput. Phys., 5 (2009), pp. 849–872.

[20] M. Ehrhardt, J. Sun, Ch. Zheng, *Evaluation of exact boundary mappings for one-dimensional semi-infinite periodic arrays*, Comm. Math. Sci., 7 (2009), pp. 347–364.

[21] J. Elschner, G.C. Hsiao, A. Rathsfeld, *An optimisation method in inverse acoustic scattering by an elastic obstacle*, SIAM J. Appl. Math., 70 (2009), pp. 168–187.

[22] J. Fuhrmann, A. Erdmann, Ch.R. Szmanda, A. Fiebach, M. Uhle, *A model of self-limiting residual acid diffusion for pattern doubling*, Microel. Engineering, 86 (2009), pp. 792–795.

[23] J. Fuhrmann, A. Linke, H. Langmach, H. Baltruschat, *Numerical calculation of the limiting current for a cylindrical thin layer flow cell*, Electrochimica Acta, 55 (2009), pp. 430–438.

[24] K. Gärtner, *Existence of bounded discrete steady state solutions of the van Roosbroeck system on boundary conforming Delaunay grids*, SIAM J. Sci. Comput., 31 (2009), pp. 1347–1362.

[25] A. Glitzky, *Energy estimates for electro-reaction-diffusion systems with partly fast kinetics*, Discrete Contin. Dyn. Syst., 25 (2009), pp. 159–174.

[26] A. Glitzky, K. Gärtner, *Energy estimates for continuous and discretized electro-reaction-diffusion systems*, Nonlinear Anal., 70 (2009), pp. 788–805.

[27] R. Henrion, Ch. Küchler, W. Römisch, *Scenario reduction in stochastic programming with respect to discrepancy distances*, Comput. Optim. Appl., 43 (2009), pp. 67–93.

[28] R. Henrion, J. Outrata, Th. Surowiec, *On the co-derivative of normal cone mappings to inequality systems*, Nonlinear Anal., 71 (2009), pp. 1213–1226.

[29] K. Hoke, H.-Chr. Kaiser, J. Rehberg, *Analyticity for some operator functions from statistical quantum mechanics*, Ann. Henri Poincare, 10 (2009), pp. 749–771.

[30] A. Fasano, D. Hömberg, L. Panizzi, *A mathematical model for case hardening of steel*, Math. Models Methods Appl. Sci., 19 (2009), pp. 2101–2126.

[31] D. Hömberg, D. Kern, *The heat treatment of steel — A mathematical control problem*, Materialwiss. Werkstofftech., 40 (2009), pp. 438–442.

[32] D. Hömberg, N. Togobytska, M. Yamamoto, *On the evaluation of dilatometer experiments*, Appl. Anal., 88 (2009), pp. 669–681.

[33] G. Hu, X. Liu, B. Zhang, *Unique determination of a perfectly conducting ball by a finite number of electric far field data*, J. Math. Anal. Appl., 352 (2009), pp. 861–871.

[34] S. Jansen, E.H. Lieb, R. Seiler, *Symmetry breaking in Laughlin's state on a cylinder*, Comm. Math. Phys., 285 (2009), pp. 503–535.

[35] V. John, T. Mitkova, M. Roland, K. Sundmacher, L. Tobiska, A. Voigt, *Simulations of population balance systems with one internal coordinate using finite element methods*, Chem. Engng. Sci., 64 (2009), pp. 733–741.

[36] H.-Chr. Kaiser, H. Neidhardt, J. Rehberg, *Classical solutions of drift-diffusion equations for semiconductor devices: The 2D case*, Nonlinear Anal., 71 (2009), pp. 1584–1605.

[37] ———, *Monotonicity properties of the quantum mechanical particle density: An elementary proof*, Monatsh. Math., 158 (2009), pp. 179–185.

[38] L. Göllmann, D. Kern, H. Maurer, *Optimal control problems with delays in state and control variables subject to mixed control-state constraints*, Optimal Control Appl. Methods, 30 (2009), pp. 341–365.

[39] P. Rudolph, M. Czupalla, N. Dropka, C. Frank-Rotsch, F.-M. Kiessling, O. Klein, B. Lux, W. Miller, U. Rehse, O. Root, *Crystal growth from melt in combined heater-magnet modules*, J. Korean Crystal Growth and Crystal Technology, 19 (2009), pp. 215–222.

[40] O. Klein, Ch. Lechner, P.-É. Druet, P. Philip, J. Sprekels, Ch. Frank-Rotsch, F.M. Kiessling, W. Miller, U. Rehse, P. Rudolph, *Numerical simulations of the influence of a traveling magnetic field, generated by an internal heater-magnet module, on liquid encapsulated Czochralski crystal growth*, Magnetohydrodynamics, 45 (2009), pp. 557–567.

[41] D. Knees, *On global spatial regularity in elasto-plasticity with linear hardening*, Calc. Var. Partial Differ. Equ., 36 (2009), pp. 611–625.

[42] W. König, H. Lacoin, P. Mörters, N. Sidorova, *A two cities theorem for the parabolic Anderson model*, Ann. Probab., 37 (2009), pp. 347–392.

[43] M. Becker, W. König, *Moments and distribution of the local times of a transient random walk on* $\mathbb{Z}^d$, J. Theoret. Probab., 22 (2009), pp. 365–374.

[44] G. Grüninger, W. König, *Potential confinement property in the parabolic Anderson model*, Ann. Inst. H. Poincare Probab. Statist., 45 (2009), pp. 840–863.

[45] V. Krätschmer, *Compactness in spaces of inner regular measures and a general Portmanteau lemma*, J. Math. Anal. Appl., 351 (2009), pp. 792–803.

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[47] P. Krejčí, M. Liero, *Rate independent Kurzweil processes*, Appl. Math., 54 (2009), pp. 117–145.

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[49] K. Kuhnen, P. Krejčí, *Compensation of complex hysteresis and creep effects in piezoelectrically actuated systems — A new Preisach modeling approach*, IEEE Trans. Autom. Control, 54 (2009), pp. 537–550.

[50] K. Krumbiegel, A. Rösch, *A virtual control concept for state constrained optimal control problems*, Comput. Optim. Appl., 43 (2009), pp. 213–233.

[51] M. Spreemann, M. Lichtner, M. Radziunas, U. Bandelow, H. Wenzel, *Measurement and simulation of distributed-feedback tapered master-oscillator power-amplifiers*, IEEE J. Quantum Electron., 45 (2009), pp. 609–616.

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[53] A. Linke, *Collision in a cross-shaped domain — A steady 2D Navier–Stokes example demonstrating the importance of mass conservation in CFD*, Comput. Methods Appl. Mech. Engrg., 198 (2009), pp. 3278–3286.

[54] R.L. Loeffen, *An optimal dividends problem with a terminal value for spectrally negative Lévy processes with a completely monotone jump density*, J. Appl. Probab., 46 (2009), pp. 85–98.

[55] ———, *An optimal dividends problem with transaction costs for spectrally negative Lévy processes*, Insurance Math. Econom., 45 (2009), pp. 41–48.

[56] B. Hoffmann, P. Mathé, H. von Weizsäcker, *Regularization in Hilbert space under unbounded operators and general source conditions*, Inverse Problems, 25 (2009), pp. 115013/1–115013/15.

[57] P. Mathé, S.V. Pereverzev, *The use of higher order finite difference schemes is not dangerous*, J. Complexity, 25 (2009), pp. 3–10.

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[10] J. Dolata, H.-J. Mucha, H.-G. Bartel, *Mapping findspots of Roman military brickstamps in* Mogontiacum *(Mainz) and archaeometrical analysis*, in: Advances in Data Analysis, Data Handling and Business Intelligence. Proceedings of the 32nd Annual Conference of the Gesellschaft für Klassifikation e.V., Joint Conference with the British Classification Society (BCS) and the Dutch/Flemish Classification Society (VOC), Helmut-Schmidt-University, Hamburg, July 16–18, 2008, A. Fink, B. Lausen, W. Seidel, A. Ultsch, eds., Studies in Classification, Data Analysis, and Knowledge Organization, Springer, Heidelberg et al.

[11] E. Haimerl, H.-J. Mucha, *Comparing the stability of clustering results of dialect data based on several distance matrices*, in: Proceedings of the 11th Conference of the International Federation of Classification Societies (IFCS 2009), Springer, Berlin.

[12] S. Bartels, R. Müller, *Die kalte Zunge*, in: Besser als Mathe — Moderne angewandte Mathematik aus dem Matheon zum Mitmachen, K. Biermann, M. Grötschel, B. Lutz-Westphal, eds., Vieweg und Teubner.

[13] H. Gross, A. Rathsfeld, M. Bär, *Modelling and uncertainty estimates for numerically reconstructed profiles in scatterometry*, in: Proceedings of the Conference on Advanced Mathematical and Computational Tools in Metrology and Testing, Paris, June 23–25, 2008.

[14] G. Schmidt, *Boundary integral methods for periodic scattering problems*, in: Around the Research of Vladimir Maz'ya II. Partial Differential Equations, A. Laptev, ed., International Mathematical Series, Springer.

A.7 Preprints, Reports

A.7.1 WIAS Preprints Series[4]

[1] V.F. Butuzov, N.N. Nefedov, L. Recke, K.R. Schneider, *Global region of attraction of a periodic solution to a singularly perturbed parabolic problem in case of exchange of stability*, Preprint no. 1432, WIAS, Berlin, 2009.

[2] L. Cherkas, A. Grin, K.R. Schneider, *On the construction of Dulac–Cherkas functions for generalized Liénard systems*, Preprint no. 1431, WIAS, Berlin, 2009.

[3] Ch. Liu, H. Wu, X. Xu, *Asymptotic behavior of a hydrodynamic system in the nematic liquid crystal flows*, Preprint no. 1401, WIAS, Berlin, 2009.

[4] S. Amiranashvili, U. Bandelow, A. Mielke, *Padé approximant for refractive index and nonlocal envelope equations*, Preprint no. 1391, WIAS, Berlin, 2009.

[5] S. Amiranashvili, A. Demircan, *Hamiltonian structure of propagation equations for ultrashort optical pulses*, Preprint no. 1472, WIAS, Berlin, 2009.

[6] I. Babushkin, *Non-Poissonian statistics in an optical analog of quantum billiard with perfectly square boundaries*, Preprint no. 1468, WIAS, Berlin, 2009.

[7] ———, *Scar-like structures and their localization in a perfectly square optical billiard*, Preprint no. 1465, WIAS, Berlin, 2009.

[8] M. Schulz-Ruhtenberg, I. Babushkin, N.A. Loiko, Th. Ackemann, K. Huang, *Polarization properties in the transition from below to above lasing threshold in broad-area vertical-cavity surface-emitting lasers*, Preprint no. 1445, WIAS, Berlin, 2009.

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

[10] G. Blanchard, G. Lee, C. Scott, *Semi-supervised novelty detection*, Preprint no. 1471, WIAS, Berlin, 2009.

[11] C. Brée, A. Demircan, S. Skupin, L. Bergé, G. Steinmeyer, *Plasma induced pulse breaking in filamentary self-compression*, Preprint no. 1453, WIAS, Berlin, 2009.

[12] W. Dreyer, S.-J. Kimmerle, *Mean field diffusion models for precipitation in crystalline GaAs including surface tension and bulk stresses*, Preprint no. 1475, WIAS, Berlin, 2009.

[13] W. Dreyer, F. Duderstadt, M. Hantke, G. Warnecke, *On phase change of a vapor bubble in liquid water*, Preprint no. 1424, WIAS, Berlin, 2009.

[14] W. Dreyer, C. Guhlke, R. Huth, *The behavior of a many particle cathode in a lithium-ion battery*, Preprint no. 1423, WIAS, Berlin, 2009.

[15] ———, *Hysteresis in the context of hydrogen storage and lithium-ion batteries*, Preprint no. 1410, WIAS, Berlin, 2009.

[16] W. Dreyer, M. Gaberšček, C. Guhlke, R. Huth, J. Jamnik, *Phase transition and hysteresis in a rechargeable lithium battery revisited*, Preprint no. 1425, WIAS, Berlin, 2009.

[17] P.-É. Druet, O. Klein, J. Sprekels, F. Tröltzsch, I. Yousept, *Optimal control of 3D state-constrained induction heating problems with nonlocal radiation effects*, Preprint no. 1422, WIAS, Berlin, 2009.

[18] M. Ehrhardt, *Absorbing boundary conditions for hyperbolic systems*, Preprint no. 1421, WIAS, Berlin, 2009.

[4] Preprints that have been written by guests during their stay at WIAS have been listed in front of those written by the collaborators of WIAS.

[19] M. Ehrhardt, Ch. Zheng, *Fast numerical methods for waves in periodic media*, Preprint no. 1441, WIAS, Berlin, 2009.

[20] ———, *Implementing exact absorbing boundary condition for the linear one-dimensional Schrödinger problem with variable potential by Titchmarsh–Weyl theory*, Preprint no. 1426, WIAS, Berlin, 2009.

[21] M. Ehrhardt, J. Fuhrmann, A. Linke, *A model of an electrochemical flow cell with porous layer*, Preprint no. 1437, WIAS, Berlin, 2009.

[22] L. Sumichrast, M. Ehrhardt, *Comparison of the continuous, semi-discrete and fully-discrete transparent boundary conditions (TBC) for the parabolic wave equation 1. Theory*, Preprint no. 1440, WIAS, Berlin, 2009.

[23] J. Elschner, M. Yamamoto, *Uniqueness in inverse elastic scattering with finitely many incident waves*, Preprint no. 1449, WIAS, Berlin, 2009.

[24] S. Chandler-Wilde, J. Elschner, *Variational approach in weighted Sobolev spaces to scattering by unbounded rough surface*, Preprint no. 1455, WIAS, Berlin, 2009.

[25] J. Elschner, G. Hu, *Variational approach to scattering of plane elastic waves by diffraction gratings*, Preprint no. 1466, WIAS, Berlin, 2009.

[26] A. Glitzky, *Uniform exponential decay of the free energy for Voronoi finite volume discretized reaction-diffusion systems*, Preprint no. 1443, WIAS, Berlin, 2009.

[27] A. Glitzky, J.A. Griepentrog, *Discrete Sobolev–Poincaré inequalities for Voronoi finite volume approximations*, Preprint no. 1429, WIAS, Berlin, 2009.

[28] J.A. Griepentrog, L. Recke, *Local existence, uniqueness, and smooth dependence for nonsmooth quasilinear parabolic problems*, Preprint no. 1409, WIAS, Berlin, 2009.

[29] H. Hanke, *Homogenization in gradient plasticity*, Preprint no. 1457, WIAS, Berlin, 2009.

[30] R. Henrion, B. Mordukhovich, N. Mau Nam, *Polyhedral systems in finite and infinite dimensions with applications to robust stability of variational inequalities*, Preprint no. 1399, WIAS, Berlin, 2009.

[31] R. Henrion, J. Outrata, Th. Surowiec, *Analysis of M-stationary points to an EPEC modeling oligopolistic competition in an electricity spot market*, Preprint no. 1433, WIAS, Berlin, 2009.

[32] ———, *Strong stationary solutions to equilibrium problems with equilibrium constraints with applications to an electricity spot market model*, Preprint no. 1396, WIAS, Berlin, 2009.

[33] D. Hömberg, A. Steinbrecher, T. Stykel, *Optimal control of robot-guided laser material treatment*, Preprint no. 1405, WIAS, Berlin, 2009.

[34] D. Hömberg, D. Kern, *The heat treatment of steel — A mathematical control problem*, Preprint no. 1402, WIAS, Berlin, 2009.

[35] V. John, M. Roland, *Simulations of 3D/4D precipitation processes in a turbulent flow field*, Preprint no. 1463, WIAS, Berlin, 2009.

[36] R. Haller-Dintelmann, H.-Chr. Kaiser, J. Rehberg, *Direct computation of elliptic singularities across anisotropic, multi-material edges*, Preprint no. 1439, WIAS, Berlin, 2009.

[37] J. Kampen, *Global analytic expansion of solution for a class of linear parabolic systems with coupling of first order derivatives terms*, Preprint no. 1398, WIAS, Berlin, 2009.

[38] D. Knees, *Global spatial regularity for time dependent elasto-plasticity and related problems*, Preprint no. 1395, WIAS, Berlin, 2009.

[39] P. Gruber, D. Knees, S. Nesenenko, M. Thomas, *Analytical and numerical aspects of time-dependent models with internal variables*, Preprint no. 1460, WIAS, Berlin, 2009.

[40] A. Bumb, D. Knees, *Global spatial regularity for a regularized elasto-plastic model*, Preprint no. 1419, WIAS, Berlin, 2009.

[41] W. König, P. Schmid, *Random walks conditioned to stay in Weyl chambers of type C and D*, Preprint no. 1461, WIAS, Berlin, 2009.

[42] M.D. Korzec, P.L. Evans, *From bell shapes to pyramids: A continuum model for self-assembled quantum dot growth*, Preprint no. 1434, WIAS, Berlin, 2009.

[43] W.K. Härdle, V. Krätschmer, R. Moro, *A microeconomic explanation of the EPK paradox*, Preprint no. 1462, WIAS, Berlin, 2009.

[44] V. Krätschmer, J.G.M. Schoenmakers, *Representations for optimal stopping under dynamic monetary utility functionals*, Preprint no. 1456, WIAS, Berlin, 2009.

[45] H. Garcke, Ch. Kraus, *An anisotropic, inhomogeneous, elastically modified Gibbs–Thomson law as singular limit of a diffuse interface model*, Preprint no. 1467, WIAS, Berlin, 2009.

[46] A. Jechow, M. Lichtner, R. Menzel, M. Radziunas, D. Skoczowsky, A.G. Vladimirov, *Stripe-array diode-laser in an off-axis external cavity: Theory and experiment*, Preprint no. 1442, WIAS, Berlin, 2009.

[47] M. Lichtner, M. Wolfrum, S. Yanchuk, *The spectrum of delay differential equations with large delay*, Preprint no. 1436, WIAS, Berlin, 2009.

[48] A. Linke, *Collision in a cross-shaped domain — A steady 2D Navier–Stokes example demonstrating the importance of mass conservation in CFD*, Preprint no. 1408, WIAS, Berlin, 2009.

[49] F. Bauer, P. Mathé, *Parameter choice methods using minimization schemes*, Preprint no. 1474, WIAS, Berlin, 2009.

[50] S. Lu, P. Mathé, *Heuristic parameter selection based on functional minimization: Optimality and model function approach*, Preprint no. 1413, WIAS, Berlin, 2009.

[51] K. Krumbiegel, Ch. Meyer, A. Rösch, *A priori error analysis for state constrained boundary control problems. Part I: Control discretization*, Preprint no. 1393, WIAS, Berlin, 2009.

[52] ———, *A priori error analysis for state constrained boundary control problems. Part II: Full discretization*, Preprint no. 1394, WIAS, Berlin, 2009.

[53] A. Mielke, *Complete-damage evolution based on energies and stresses*, Preprint no. 1414, WIAS, Berlin, 2009.

[54] ———, *Differential, energetic, and metric formulations for rate-independent processes*, Preprint no. 1454, WIAS, Berlin, 2009.

[55] J. Giannoulis, A. Mielke, Ch. Sparber, *High-frequency averaging in semi-classical Hartree-type equations*, Preprint no. 1447, WIAS, Berlin, 2009.

[56] A. Mielke, C. Patz, *Dispersive stability of infinite dimensional Hamiltonian systems on lattices*, Preprint no. 1448, WIAS, Berlin, 2009.

[57] A. Mielke, R. Rossi, G. Savaré, *BV solutions and viscosity approximations of rate-independent systems*, Preprint no. 1451, WIAS, Berlin, 2009.

[58] A. Mielke, U. Stefanelli, *Weighted energy-dissipation functionals for gradient flows*, Preprint no. 1400, WIAS, Berlin, 2009.

[59] A. Mielke, L. Paoli, A. Petrov, U. Stefanelli, *Error estimates for space-time discretizations of a rate-independent variational inequality*, Preprint no. 1407, WIAS, Berlin, 2009.

[60] M. Thomas, A. Mielke, *Damage of nonlinearly elastic materials at small strain — Existence and regularity results*, Preprint no. 1397, WIAS, Berlin, 2009.

[61] S. Bartels, R. Müller, *Optimal and robust a posteriori error estimates in $L^\infty(L^2)$ for the approximation of Allen–Cahn equations past singularities*, Preprint no. 1416, WIAS, Berlin, 2009.

[62] M. Jensen, R. Müller, *Stable Crank–Nicolson discretisation for incompressible miscible displacement problems of low regularity*, Preprint no. 1450, WIAS, Berlin, 2009.

[63] J. Behrndt, M.M. Malamud, H. Neidhardt, *Finite rank perturbations, scattering matrices and inverse problems*, Preprint no. 1406, WIAS, Berlin, 2009.

[64] P. Exner, H. Neidhardt, *Trotter–Kato product formula for unitary groups*, Preprint no. 1428, WIAS, Berlin, 2009.

[65] M.M. Malamud, H. Neidhardt, *On the unitary equivalence of absolutely continuous parts of self-adjoint extensions*, Preprint no. 1427, WIAS, Berlin, 2009.

[66] D. Peschka, A. Münch, B. Niethammer, *Self-similar rupture of viscous thin films in the strong-slip regime*, Preprint no. 1418, WIAS, Berlin, 2009.

[67] ———, *Thin film rupture for large slip*, Preprint no. 1417, WIAS, Berlin, 2009.

[68] J. Polzehl, K. Tabelow, *Structural adaptive smoothing: Principles and applications in imaging*, Preprint no. 1412, WIAS, Berlin, 2009.

[69] P.N. Racec, R. Racec, H. Neidhardt, *R-matrix formalism for electron scattering in two dimensions*, Preprint no. 1452, WIAS, Berlin, 2009.

[70] R. Čiegis, I. Laukaitytė, M. Radziunas, *Numerical algorithms for Schrödinger equation with artificial boundary conditions*, Preprint no. 1446, WIAS, Berlin, 2009.

[71] H. Gross, A. Rathsfeld, F. Scholze, M. Bär, *Profile reconstruction in EUV scatterometry: Modeling and uncertainty estimates*, Preprint no. 1411, WIAS, Berlin, 2009.

[72] R. Haller-Dintelmann, J. Rehberg, *Coercivity for elliptic operators and positivity of solutions on Lipschitz domains*, Preprint no. 1473, WIAS, Berlin, 2009.

[73] ———, *Maximal parabolic regularity for divergence operators on distribution spaces*, Preprint no. 1459, WIAS, Berlin, 2009.

[74] O. Rott, E. Jarlebring, *An iterative method for the multipliers of periodic delay-differential equations and the analysis of a PDE milling model*, Preprint no. 1470, WIAS, Berlin, 2009.

[75] R. Schlundt, F.-J. Schmückle, W. Heinrich, *Shifted linear systems in electromagnetics. Part I: Systems with identical right-hand sides*, Preprint no. 1420, WIAS, Berlin, 2009.

[76] G. Schmidt, *Integral methods for conical diffraction*, Preprint no. 1435, WIAS, Berlin, 2009.

[77] L.I. Goray, G. Schmidt, *Solving conical diffraction with integral equations*, Preprint no. 1469, WIAS, Berlin, 2009.

[78] F. Lanzara, V. Maz'ya, G. Schmidt, *Tensor product approximations of high dimensional potentials*, Preprint no. 1403, WIAS, Berlin, 2009.

[79] J.G.M. Schoenmakers, *The real multiple dual*, Preprint no. 1438, WIAS, Berlin, 2009.

[80] V. Spokoiny, *Parameter estimation in time series analysis*, Preprint no. 1404, WIAS, Berlin, 2009.

[81] P. Krejčí, J. Sprekels, H. Wu, *Elastoplastic Timoshenko beams*, Preprint no. 1430, WIAS, Berlin, 2009.

[82] V.Z. Tronciu, M. Lichtner, M. Radziunas, U. Bandelow, H. Wenzel, *Improving the stability of distributed-feedback tapered master-oscillator power-amplifiers*, Preprint no. 1444, WIAS, Berlin, 2009.

[83] A.G. Vladimirov, A. Pimenov, D. Rachinskii, *Bifurcations in a model of monolithic passively mode-locked semiconductor laser*, Preprint no. 1458, WIAS, Berlin, 2009.

[84] W. Wagner, *Random and deterministic fragmentation models*, Preprint no. 1464, WIAS, Berlin, 2009.

[85] A. Weiss, *Executing large orders in a microscopic market model*, Preprint no. 1415, WIAS, Berlin, 2009.

A.7.2 WIAS Reports Series

[1] H.-J. Mucha, G. Ritter, *Classification and clustering: Models, software and applications*, WIAS Report no. 26, WIAS, Berlin, 2009.

A.7.3 Preprints/Reports in other Institutions

[1] P. Friz, M. Caruana, H. Oberhauser, *A (rough) pathwise approach to fully non-linear stochastic partial differential equations*, RICAM Report no. 2009-03, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, 2009.

[2] I. Babushkin, *Scar-like structures and non-integrability in a perfectly square optical billiard (electronic only)*, arXiv:0909.4330, Cornell University Library, arXiv.org, Ithaca, USA, 2009.

[3] M. Schulz-Ruhtenberg, I. Babushkin, N.A. Loiko, K.F. Huang, T. Ackemann, *Polarization properties in the transition from below to above lasing threshold in broad-area vertical-cavity surface-emitting lasers (electronic only)*, arXiv:0909.3812, Cornell University Library, arXiv.org, Ithaca, USA, 2009.

[4] S. Arlot, G. Blanchard, E. Roquain, *Some non-asymptotic results on resampling in high dimension, I: Confidence regions, II: Multiple tests (electronic only)*, arXiv:0712.0775, Cornell University Library, arXiv.org, Ithaca, USA, 2009.

[5] J. Kampen, *On the multivariate Burgers equation and the incompressible Navier–Stokes equation (electronic only)*, arXiv:0910.5672, Cornell University Library, arXiv.org, Ithaca, USA, 2009.

[6] P. Krejčí, E. Rocca, J. Sprekels, *Phase separation in a gravity field (electronic only)*, arXiv:0905.2131, Cornell University Library, arXiv.org, Ithaca, USA, 2009.

[7] F. Klopp, B. Metzger, *The Gross–Pitaevskii functional with a random background potential and condensation in the single particle ground state*, arXiv:0910.2896, Cornell University Library, arXiv.org, Ithaca, USA, 2009.

[8] S. Bartels, R. Müller, *Error controlled local resolution of evolving interfaces for generalized Cahn-Hilliard equations*, Preprint no. 09–02, Humboldt-Universität zu Berlin, Institut für Mathematik, 2009.

[9] F. Lanzara, V. Maz'ya, G. Schmidt, *On the fast computation of high dimensional volume potentials (electronic only)*, arXiv:0911.0443, Cornell University Library, arXiv.org, Ithaca, USA, 2009.

[10] P. Colli, G. Gilardi, P. Podio-Guidugli, J. Sprekels, *Global solution and long-time behavior for a problem of phase segregation of the Allen–Cahn type (electronic only)*, arXiv:0902.4741, Cornell University Library, arXiv.org, Ithaca, USA, 2009.

[11] P. Perlikowski, S. Yanchuk, M. Wolfrum, A. Stefanski, P. Mosiolek, T. Kapitaniak, *Routes to complex dynamics in a ring of unidirectionally coupled systems*, Preprint no. 667, DFG Research Center Matheon, Berlin, 2009.

A.8 Talks, Posters, and Contributions to Exhibitions[5]

A.8.1 Main Talks

1. P. Friz, *From numerical aspects of stochastic financial models to the foundations of stochastic differential equations (and back)*, Annual Meeting of the Deutsche Mathematiker-Vereinigung and 17th Congress of the Österreichische Mathematische Gesellschaft, section "Financial and Actuarial Mathematics", September 20–25, Technische Universität Graz, Austria, September 25.
2. W. Dreyer, *Phase transitions during hydrogen storage and in lithium-ion batteries*, EUROTHERM Seminar no. 84: Thermodynamics of Phase Changes, May 25–27, Université Catholique de Louvain, Namur, Belgium, May 27.
3. J. Fuhrmann, *Mathematical and numerical models of electrochemical processes related to porous media*, International Conference on Non-linearities and Upscaling in Porous Media (NUPUS), October 5–7, Universität Stuttgart, October 6.
4. R. Henrion, *Characterization of M-stationary points for an equilibrium problem in an electricity spot market model*, 16th International Conference on Mathematical Methods in Economics and Industry, June 15–18, České Budějovice, Czech Republic, June 17.
5. A. Mielke, *Multiscale modeling for energy-driven systems*, Workshop on Scale Transitions in Space and Time for Materials, October 19–23, Lorentz Center, Leiden, The Netherlands, October 19.
6. W. Wagner, *Random and deterministic fragmentation models*, Seventh IMACS Seminar on Monte Carlo Methods (MCM2009), September 6–11, Université Libre de Bruxelles, Brussels, Belgium, September 7.

A.8.2 Scientific Talks (Invited)

1. P. Friz, *Rough paths and the gap between deterministic and stochastic differential equations*, Berlin Mathematical School, Friday Colloquium, December 18.
2. S. Amiranashvili, *Modeling of ultrashort optical pulses*, Workshop "Pulses and Modulations in Nonlinear Systems", February 25–27, Universität Stuttgart, February 26.
3. I. Babushkin, *Nonresonant frequency conversion with ultrashort intense pulses in hollow microcapillaries*, University of Bath, Department of Physics, UK, December 9.
4. U. Bandelow, *3D semiclassical multi-species modeling of QD lasers*, International Nano-Optoelectronic Workshop (iNOW 2009), August 2–15, Royal Institute of Technology/Technical University of Berlin, Stockholm/Berlin, Sweden/Germany, August 14.
5. ———, *Semiconductor laser instabilities and dynamics (short course)*, 9th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD) 2009, September 14–18, Gwangju Institute of Science and Technology (GIST), Republic of Korea, September 16.
6. ———, *Mathematical models for ultrashort optical pulses*, Australasian Conference on Optics, Lasers and Spectroscopy and Australian Conference on Optical Fibre Technology in association with the International Workshop on Dissipative Solitons (ACOLS ACOFT DS 2009), November 29 – December 3, University of Adelaide, Australia, November 30.
7. ———, *Nonlinear and nonlocal models for ultrashort optical pulses*, Fourth 'Rio de la Plata' Workshop on Laser Dynamics and Nonlinear Photonics, December 8–11, Piriapolis, Uruguay, December 9.

[5] Contributions by scholarship holders and guests during their stay at WIAS have been listed in front of those made by the collaborators of WIAS.

8. D. Belomestny, *Estimation of the jump activity of a Lévy process from low frequency data*, Haindorf Seminar 2009, February 12–15, Humboldt-Universität zu Berlin, CASE – Center for Applied Statistics and Economics, Hejnice, Czech Republic, February 12.
9. ———, *Spectral estimation of the fractional order of a Lévy process*, Workshop "Statistical Inference for Lévy Processes with Applications to Finance", July 15–17, EURANDOM, Eindhoven, The Netherlands, July 16.
10. A. Bianchi, *Coupling in potential wells: From average to pointwise estimates of metastable times*, EURANDOM, Eindhoven, The Netherlands, February 18.
11. ———, *Coupling in potential wells: From average to pointwise estimates of metastable times*, BRG Workshop on Stochastic Models from Biology and Physics, April 2–4, Rheinische Friedrich-Wilhelms-Universität, Institut für Angewandte Mathematik, Bonn, April 2.
12. ———, *Coupling in potential wells: From average to pointwise estimates of metastable times*, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, May 5.
13. ———, *Gibbs specifications and Gibbs measures. The Gaussian case (tutorial session)*, Summer School in Probability, July 6–10, Università di Bologna, Italy, July 6.
14. ———, *Elements of stochastic processes theory. The generator of a process, the Poisson equation and its solution, continuous time random walks (tutorial session)*, Summer School in Probability, July 6–10, Università di Bologna, Italy, July 7.
15. M. Birkner, J. Blath, *Measure-valued diffusions, general coalescents, and population genetic inference*, Workshop "Random Trees", January 18–24, Mathematisches Forschungsinstitut Oberwolfach, January 20.
16. G. Blanchard, *Convergence du gradient conjugué fonctionnel pour l'apprentissage statistique*, École Normale Supérieure, Paris, France, March 16.
17. ———, *Non-asymptotic adaptive control of the family-wise error rate in multiple testing*, Journées Statistiques du Sud 2009, June 17–19, Université de Provence Aix-Marseille I, Porquerolles, France, June 17.
18. W. Dreyer, *Sharp interface limits of phase field models in the context of liquid-vapor transitions*, Fourth Workshop "Micro-Macro Modelling and Simulation of Liquid-Vapour Flows", February 4–6, Rheinisch-Westfälische Technische Hochschule Aachen, February 6.
19. ———, *Substitution of the Navier–Stokes–Korteweg model by a phase field model with an artificial phase field*, Meeting of the DFG-CNRS Research Unit 563 "Micro-Macro Modelling and Simulation of Liquid-Vapour Flows", March 16–17, Universität Freiburg, March 16.
20. ———, *Über Kristalle zur Speicherung von Wasserstoff und von Lithium in Lithium-Ionen-Batterien*, 6. Workshop Angewandte Simulation in der Kristallzüchtung, April 1–3, Griebnitzsee, April 2.
21. ———, *On a paradox within the phase field modeling of storage systems and its resolution*, PF09 – 2nd Symposium on Phase-Field Modelling in Materials Science, August 30 – September 2, Universität Aachen, Kerkrade, The Netherlands, August 31.
22. ———, *Modeling and simulation of the storage problem for rechargeable lithium-ion batteries*, Kick-off Meeting to start the DFG Priority Program WeNDeLIB, Universität Bochum, September 7.
23. ———, *Stochastic evolution of many particle storage systems*, 9th Hirschegg Workshop on Conservation Laws, September 6–12, Hirschegg, September 10.
24. ———, *Phase field models and their sharp limits in the context of hydrogen storage and lithium-ion batteries*, 1st International Conference on Material Modelling (1st ICMM), September 15–18, Technische Universität Dortmund, September 16.

25. ———, *Phase transitions and kinetic relations*, Séminaire Fluides Compressibles, Université Pierre et Marie Curie, Laboratoire Jacques-Louis Lions, Paris, France, September 30.

26. ———, *Phase transitions with sharp interfaces and corresponding phase field models*, Seminar of the International Research Training Group "Mathematical Fluid Dynamics", Technische Universität Darmstadt, October 15.

27. ———, *Thermodynamics of phase transitions*, Technische Universität Darmstadt, Center of Smart Interfaces (CSI), October 15.

28. ———, *Hysteresis due to non-monotone material behavior inside many-particle cathodes*, Max-Planck-Institut für Festkörperphysik, Stuttgart, December 9.

29. P.-É. Druet, *Higher integrability of the magnetic field for 3D induction heating and MHD problems*, 14th Belgian-French-German Conference on Optimization, September 14–18, Leuven, Belgium, September 15.

30. M. Ehrhardt, *Numerical simulation of periodic structure problems*, Minisymposium "Transparent Boundary Conditions", Konrad-Zuse-Zentrum für Informationstechnik Berlin, January 19.

31. ———, *A high order finite element method for waves in periodic structures*, 9th International Conference on Spectral and High Order Methods (ICOSAHOM09), Minisymposium "High-order Methods for Linear and Nonlinear Wave Equations", June 22–26, Norwegian University of Science and Technology, Trondheim, June 24.

32. ———, *The fluid-porous interface problem: Analytic and numerical solutions to flow cell problems*, Mathematical Models in Medicine, Business, Engineering (XI JORNADAS IMM), September 8–11, Technical University of Valencia, Institute of Multidisciplinary Mathematics, Spain, September 10.

33. J. Elschner, *Direct and inverse problems in fluid-solid interaction*, University of Tokyo, Department of Mathematical Sciences, February 13.

34. ———, *On uniqueness in inverse elastic scattering*, Workshop on Advances and Trends in Integral Equations, October 5–9, Klaffenbach, October 7.

35. J. Fuhrmann, *Numerical modeling in electrochemistry*, Conference on Scientific Computing (ALGORITMY 2009), March 15–20, Slovak University of Technology, Department of Mathematics and Descriptive Geometry, Podbanské, March 17.

36. ———, *Modeling of reaction diffusion problems in semiconductor photoresists*, Seventh Negev Applied Mathematical Workshop, July 6–8, Ben Gurion University of the Negev, Jacob Blaustein Institute for Desert Research, Sede Boqer Campus, Israel, July 8.

37. ———, *Reaction-diffusion processes in polymer resists*, Workshop "Evolution Equations, Related Topics and Applications", September 7–11, Helmholz-Zentrum München, September 8.

38. ———, *Mathematical and numerical modeling of fuel cells and electrochemical flow cells*, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern, December 1.

39. A. Glitzky, *Discrete Sobolev–Poincaré inequalities for finite volume Voronoi approximations*, Annual Meeting of the Deutsche Mathematiker-Vereinigung and 17th Congress of the Österreichische Mathematische Gesellschaft, section "Partial Differential Equations", September 20–25, Technische Universität Graz, Austria, September 21.

40. ———, *Discrete Sobolev–Poincaré inequalities using the $W^{1,p}$ seminorm in the setting of Voronoi finite volume approximations*, International Conference on Elliptic and Parabolic Equations, November 30 – December 4, WIAS, December 3.

41. H. Hanke, *Gamma-limits in rate-independent evolutionary problems and homogenization in gradient plasticity*, DK-Seminar "Numerical Simulations in Technical Sciences", Graz University of Technology, Faculty of Technical Mathematics and Technical Physics, Austria, November 18.

42. R. Henrion, *A model for dynamic chance constraints in water reservoir management*, 23rd European Conference on Operational Research (EURO23), July 6–8, Bonn, July 7.

43. ———, *On stationarity conditions for an equilibrium problem with equilibrium constraints from an electricity spot market model*, 23rd European Conference on Operational Research (EURO23), July 6–8, Bonn, July 7.

44. ———, *Answers and questions in selected topics of probabilistic programming*, International Colloquium on Stochastic Modeling and Optimization, November 30 – December 1, Rutgers University, New Brunswick, USA, November 30.

45. K. Hoke, *Hartree solution of the Kohn–Sham system for semiconductor devices*, Berlin-Leipzig Seminar on Numerics, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, March 18.

46. ———, *Iterative solution of the Kohn–Sham system for semiconductor devices*, International Conference "Mathematics of Finite Elements and Applications 2009 (MAFELAP)", minisymposium "Numerical Problems in Density Functional Theory", June 9–12, The Brunel Institute of Computational Mathematics (BICOM), Uxbridge, UK, June 12.

47. D. Hömberg, *Die Wärmebehandlung von Stahl — Thermomechanische Modellierung, Simulation und Optimierung*, Technische Universität Dortmund, Fakultät Maschinenbau, January 22.

48. ———, *Coupling of process, machine, and work-piece in production processes — A challenge for industrial mathematics*, Workshop "Industrial Mathematics and its Practice", February 23–24, University of Tokyo, Japan, February 23.

49. ———, *Direct and inverse problems related to phase transitions and distortion in modern multi-phase steels*, Workshop "Mathematical Models and Analytical Problems for Special Materials", July 9–11, Università degli Studi di Brescia, Italy, July 9.

50. ———, *Distortion compensation — An optimal control approach*, 24th IFIP TC 7 Conference on System Modelling and Optimization, July 27–31, Buenos Aires, Argentina, July 27.

51. ———, *The mathematics of distortion*, University of Delaware, Department of Mathematical Sciences, Newark, USA, October 6.

52. ———, *Optimal control of heat treatments and stability of milling processes — Two case studies from industrial mathematics*, Worcester Polytechnic Institute, Mechanical Engineering Department, USA, October 7.

53. ———, *Interactions between machine, work-piece, and process dynamics in milling machines*, SIAM Conference on Mathematics for Industry: Challenges and Frontiers (MI09), October 9–10, San Francisco, USA, October 9.

54. V. John, *A variational multiscale method for turbulent flow simulation with adaptive large scale space*, Workshop on Computational Multiscale Modeling, November 26–27, University of Twente, Enschede, The Netherlands, November 27.

55. ———, *On the numerical simulation of population balance systems*, Karlsruher Institut für Technologie, Fakultät für Mathematik, December 9.

56. G. Kitavtsev, *Reduced ODE models describing coarsening dynamics of slipping droplets and a geometrical approach for their derivation*, Oberseminar, Universität Bonn, Institut für Angewandte Mathematik, July 23.

57. ———, *Reduced ODE models describing coarsening dynamics of slipping droplets*, Oberseminar Analysis, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, October 30.

58. D. Knees, *Crack propagation in polyconvex materials*, Colloquium Dedicated to A.M. Sändig's 65th Birthday, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, July 17.

59. ———, *On the inviscid limit of a model for crack propagation*, Multiscale Asymptotics and Computational Approximation for Surface Defects and Applications in Mechanics (MACADAM), August 31 – September 1, Ecole Normale Supérieure de Cachan, France, August 31.

60. ———, *On quasistatic crack propagation in finite-strain elasticity*, University of Pavia, Institute of Applied Mathematics and Information Technology (IMATI), Italy, September 8.

61. ———, *On global spatial regularity in elasto-plasticity*, Seminar "Numerische Mathematik", Graz University of Technology, Faculty of Technical Mathematics and Technical Physics, Austria, October 29.

62. ———, *On global spatial regularity in elasto-plasticity*, International Conference on Elliptic and Parabolic Equations, November 30 – December 4, WIAS, December 4.

63. W. König, *Phase transitions for dilute particle systems with Lennard–Jones potential*, Workshop on Mathematics of Phase Transitions: Past, Present, Future, November 12–15, University of Warwick, Coventry, UK, November 15.

64. P. Krejčí, *Oscillations of elastoplastic beams and plates*, Oberseminar Analysis, Technische Universität München, Zentrum Mathematik, January 22.

65. ———, *Phase transitions in an elastoplastic container*, Equazioni alle Derivate Parziali Modelli e Applicazioni, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, March 24.

66. K. Krumbiegel, *Optimalsteuerung mit Zustandsbeschränkungen*, Universität Leipzig, Fakultät für Mathematik und Informatik, October 6.

67. A. Linke, *The discretization of coupled flows and the problem of mass conservation*, Workshop on Discretization Methods for Viscous Flows, Part II: Compressible and Incompressible Flows, June 24–26, Porquerolles, Toulon, France, June 25.

68. A. Linke, *The discretization of coupled flows and the problem of mass conservation*, Seventh Negev Applied Mathematical Workshop, July 6–8, Ben Gurion University of the Negev, Jacob Blaustein Institute for Desert Research, Sede Boqer Campus, Israel, July 7.

69. ———, *Divergence-free mixed finite elements for the incompressible Navier–Stokes equations*, Universität Stuttgart, Institut für Wasserbau, December 8.

70. R. Loeffen, *De Finetti's optimal dividends problem with an affine penalty function at ruin*, Université Libre de Bruxelles, Département de Mathématiques, Belgium, November 19.

71. P. Mathé, *Typical behavior in heuristic parameter choice*, Kick-Off Meeting of Mini Special Semester on Inverse Problems, May 18–22, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, May 18.

72. ———, *Discretization under general smoothness assumptions*, Monday Lecture Series, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, June 29.

73. ———, *On some minimization-based heuristic parameter choice in inverse problems*, Chemnitz-RICAM Symposium on Inverse Problems, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, July 14.

74. ———, *Approximation theoretic aspects in variable Hilbert scales*, 2nd Dolomites Workshop on Constructive Approximation and Applications, September 3–10, Università degli Studi di Verona, Dipartimento di Informatica, Italy, September 5.

75. ———, *Inverse problems in different settings*, Seminar "Algorithms and Complexity for Continuous Problems", September 20–25, Schloss Dagstuhl, September 25.

76. B. Metzger, *The discrete Gross–Pitaevskii model and condensation in the single particle ground state*, Berlin-Leipzig Seminar on Analysis and Probability Theory, Technische Universität Berlin, Institut für Mathematik, November 27.

77. Ch. Meyer, *Finite element error analysis for state-constrained optimal control of the Stokes problem*, 80th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2009), section "Optimization of Differential Equations", February 9–13, Gdansk University of Technology, Poland, February 10.

78. A. Mielke, *Geometrische Nichtlinearitäten und Lie-Gruppen in der Elastoplastizität*, Mathematisches Kolloquium, Universität Paderborn, Institut für Mathematik, January 27.

79. ———, *BV solutions and parametrized solutions for rate-independent systems*, 80th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2009), session "Applied Analysis", February 9–13, Gdansk University of Technology, Poland, February 10.

80. ———, *Modeling the evolution of complete damage via parametrized Gamma-convergence*, International Workshop on Phase Transitions — Phase Variations 2009, May 21–22, Università di Pavia, Dipartimento di Matematica, Italy, May 22.

81. ———, *Vanishing-viscosity solutions for rate-independent energetic system*, Workshop on Energy-Driven Systems, August 27–29, Carnegie Mellon University, Center for Nonlinear Analysis, Pittsburgh, USA, August 27.

82. ———, *Homogenization via Gamma-convergence for hyperbolic problems*, Workshop "The Future for Complexity Sciences", September 15–16, University of Bath, Department of Mathematical Sciences, UK, September 15.

83. ———, *Parabolic equations in the vanishing-viscosity limit*, International Conference on Elliptic and Parabolic Equations, November 30 – December 4, WIAS, December 4.

84. ———, *Vanishing-viscosity approximation of rate-independent systems*, Workshop "Material Theories", December 14–18, Mathematisches Forschungsinstitut Oberwolfach, December 15.

85. H.-J. Mucha, *Clustering accompanied by visualization and validation*, 11th Conference of the International Federation of Classification Societies (IFCS 2009), March 13–18, Technische Universität Dresden, March 13.

86. ———, *Explorative statistische Methoden in der Archäometrie: von Daten zu Distanzen und weiter zu Gruppierungen*, Curt-Engelhorn-Zentrum Archäometrie Mannheim, July 9.

87. H. Neidhardt, *Sturm–Liouville operators with operator potentials*, Quantum Circle Seminar, Doppler Institute for Mathematical Physics and Applied Mathematics, Czech Technical University, Prague, March 17.

88. ———, *On carrier transport modeling in semiconductor devices at WIAS: A survey*, Satellite Meeting of the International Congress of Mathematical Physics "Mathematical Aspects of Quantum Transport and Applications in Nanophysics", August 10–13, Aalborg University, Department of Mathematical Sciences, Denmark, August 10.

89. ———, *Linear non-autonomous Cauchy problems and evolution semigroups*, International Bogolyubov Conference "Problems of Theoretical and Mathematical Physics", August 21–27, Moscow State University/Joint Institute for Nuclear Research, Dubna, Russia, August 24.

90. ———, *On the Kato–Rosenblum and the Weyl–von Neumann theorem for self-adjoint extensions of symmetric operators*, Séminaire de Physique Statistique & Matière Condensée, Centre National de la Recherche Scientifique Luminy, Centre de Physique Théorique, Marseille, France, October 7.

91. C. Patz, *Propagation of wave fronts in Hamiltonian systems on infinite lattices*, Workshop on Pulses and Modulations in Nonlinear Systems, February 25–27, Universität Stuttgart, Institut für Analysis, Dynamik und Modellierung, February 26.

92. D. Peschka, *Self-similar rupture for thin films with slip*, EUROMECH Colloquium 497 — Recent Developments and New Directions in Thin-Film Flow, July 6–9, Royal Society of Edinburgh, UK, July 8.

93. A. Petrov, *On the existence and error bounds for space-time discretizations of a 3D model for shape-memory alloys*, Lisbon University, Center for Mathematics and Fundamental Applications, Portugal, September 17.

94. J. Polzehl, *Sequential multiscale procedures for adaptive estimation*, The 1st Institute of Mathematical Statistics Asia Pacific Rim Meeting, June 28 – July 1, Seoul National University, Institute of Mathematical Statistics, Seoul, Korea, July 1.

95. P.N. Racec, *Evanescent channels and scattering in cylindrical nanowire heterostructures*, Physikalisches Kolloquium, Brandenburgische Technische Universität Cottbus, April 14.

96. ———, *Quantum transport in cylindrical nanowire heterostructures: The scattering problem*, Paul-Drude-Institut für Festkörperelektronik, Abteilung Epitaxie, Berlin, May 13.

97. P.N. Racec, *Scattering theory in cylindrical nanowire heterostructures*, Seminar of Nonequilibrium Many-Body Systems Group, Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, December 7.

98. M. Radziunas, *Simulation and analysis of longitudinal dynamics in semiconductor laser devices*, Tyndall National Institute, Photonics Theory Group, Cork, Ireland, June 25.

99. A. Rathsfeld, *Modelling and algorithms for simulation and reconstruction in scatterometry*, Seminar on Scatterometry and Ellipsometry on Structured Surfaces, March 18–19, Physikalisch-Technische Bundesanstalt Braunschweig, March 18.

100. ———, *Numerical aspects of the scatterometric measurement of periodic surface structures*, Conference on Applied Inverse Problems 2009, July 20–24, University of Vienna, Austria, July 21.

101. ———, *Numerical solution of an inverse scattering problem by an elastic obstacle*, Workshop on Advances and Trends in Integral Equations, October 5–9, Klaffenbach, October 7.

102. J. Rehberg, *Functional analytic properties of the quantum mechanical particle density operator*, International Workshop on Quantum Systems and Semiconductor Devices: Analysis, Simulations, Applications, April 20–24, Peking University, School of Mathematical Sciences, Beijing, China, April 21.

103. ———, *Quasilinear parabolic equations in distribution spaces*, International Conference on Nonlinear Parabolic Problems in Honor of Herbert Amann, May 10–16, Stefan Banach International Mathematical Center, Bedlewo, Poland, May 12.

104. G. Schmidt, *Boundary integral methods for periodic scattering problems*, Workshop on Advances and Trends in Integral Equations, October 5–9, Klaffenbach, October 7.

105. ———, *Boundary integral methods for periodic scattering problems*, University of Liverpool, Department of Mathematics, UK, October 14.

106. J.G.M. Schoenmakers, *Monte Carlo methods for pricing of complex structured callable derivatives*, Rhein-Main Arbeitskreis *Mathematics of Computation*, Johann Wolfgang Goethe-Universität Frankfurt, Villa Giersch, January 16.

107. ———, *Holomorphic transforms with application to affine processes*, Workshop “Computational Finance”, August 10–12, Kyoto University, Faculty of Sciences, Japan, August 10.

108. ———, *Regression methods for stochastic control problems and their convergence analysis*, Workshop “Computational Finance”, August 10–12, Kyoto University, Faculty of Sciences, Japan, August 10.

109. V. Spokoiny, *Modern nonparametric statistics (block lecture)*, 4 talks, École Nationale de la Statistique et de l’Analyse de l’Information (ENSAI), Rennes, France, January 13–16.

110. ———, *Adaptive local parametric methods in imaging*, Technische Universität Kaiserslautern, Fachbereich Mathematik, January 23.

111. ———, *Adaptive local parametric estimation*, Université Joseph Fourier Grenoble I, Équipe de Statistique et Modélisation Stochastique, Laboratoire Jean Kuntzmann, France, February 26.

112. ———, *Sparse non-Gaussian component analysis*, Workshop "Sparse Recovery Problems in High Dimensions: Statistical Inference and Learning Theory", March 15–21, Mathematisches Forschungsinstitut Oberwolfach, March 16.

113. ———, *Non-Gaussian component analysis*, Workshop "Semiparametric and Nonparametric Methods in Econometrics", April 4–11, Banff International Research Station for Mathematical Innovation and Discovery, Canada, April 6.

114. ———, *Parameter tuning in statistical inverse problem*, European Meeting of Statisticians (EMS2009), July 20–22, Université Paul Sabatier, Toulouse, France, July 21.

115. ———, *Saddle point model selection for inverse problems*, Workshop "Challenges in Statistical Theory: Complex Data Structures and Algorithmic Optimization", August 23–29, Mathematisches Forschungsinstitut Oberwolfach, August 26.

116. ———, *Modern nonparametric statistics (block lecture)*, 4 talks, École Nationale de la Statistique et de l'Analyse de l'Information (ENSAI), Rennes, France, October 2–13.

117. ———, *Modern nonparametric statistics (block lecture)*, 4 talks, Yale University, New Haven, USA, October 18–29.

118. ———, *Saddle point model selection*, 2nd Humboldt-Princeton Conference: Perceiving and Measuring Financial Risk: Credit, Energy and Illiquidity, October 30–31, Princeton University, USA, October 30.

119. ———, *Saddle point model selection*, Université Toulouse 1 Capitole, Toulouse School of Economics, France, November 24.

120. ———, *Cross concentration in semiparametric estimation*, Rencontres de Statistiques Mathématiques 9, December 14–18, International Center for Mathematical Meetings (CIRM), Marseille, France, December 15.

121. J. Sprekels, *Problems in the industrial growth of semiconductor crystals: Radiative transfer, convection, magnetic fields, and free boundaries*, Seminar of the Institute of Applied Mathematics and Information Technology, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, September 23.

122. ———, *Mathematik — mehr als nur die Sprache der Natur. Beiträge zu den Materialwissenschaften*, Herbsttagung (Autumn Meeting) 2009, Mathematische Gesellschaft in Hamburg, November 6–7, November 6.

123. K. Tabelow, *Structural adaptive smoothing in fMRI and DTI*, Workshop on Recent Developments in fMRI Analysis Methods, Bernstein Center for Computational Neuroscience Berlin, January 23.

124. ———, *Structural adaptive methods in fMRI and DTI*, Biomedical Imaging Research Seminar Series, Weill Cornell Medical College, Department of Radiology & Citigroup Biomedical Imaging Center, New York, USA, June 25.

125. ———, *Structural adaptive methods in fMRI and DTI*, Memorial Sloan-Kettering Cancer Center, New York, USA, June 25.

126. N. Togobytska, *Parameter identification for the phase transformations in steel*, Conference on Applied Inverse Problems 2009, July 20–24, University of Vienna, Austria, July 21.

127. V.Z. Tronciu, *Chaos based communication using multi-section semiconductor laser*, Seminar of the DFG Collaborative Research Center (SFB) 787 "Semiconductor Nanophotonics: Materials, Models, Devices", Technische Universität Berlin, May 14.

128. ———, *Numerical simulations of DFB-MOPA and DBR tapered power-amplifiers*, Photo Meeting, University of the Balearic Islands, Institute for Cross-Disciplinary Physics and Complex Systems (IFISC), Palma de Mallorca, Spain, June 26.

129. ———, *Numerical simulations of DFB-MOPA and DBR tapered power-amplifiers*, Universidad Politécnica de Madrid, Departamento de Tecnología Fotónica, Spain, June 29.

130. ———, *Dynamics of DFB tapered master-oscillator power-amplifiers. Applications*, Seminar of the Laboratory of Theory of Semiconductors and Quantum Electronics, Academy of Sciences of Moldova, Institute of Applied Physics, Chisinau, October 9.

131. A.G. Vladimirov, *Spontaneous motion of dissipative solitons under the effect of delay*, Australasian Conference on Optics, Lasers and Spectroscopy and Australian Conference on Optical Fibre Technology in association with the International Workshop on Dissipative Solitons (ACOLS ACOFT DS 2009), November 29 – December 3, University of Adelaide, Australia, December 1.

132. B. Wagner, *Influence of slip on droplet dynamics*, British Applied Mathematics Colloquium 2009, April 7–9, University of Nottingham, UK, April 7.

133. W. Wagner, *Fragmentation equations and stochastic models*, Workshop "Asymptotic Methods for Dissipative Particle Systems", May 18–22, University of California, Institute for Pure and Applied Mathematics, Los Angeles, USA, May 18.

134. ———, *Fragmentation models*, Workshop on Theory and Applications of Classical and Quantum Kinetic Theory, June 21–26, Banff International Research Station for Mathematical Innovation and Discovery, Canada, June 23.

135. ———, *Introduction to Markov jump processes*, Scuola Superiore di Catania, Laboratory for Complex Systems, Italy, October 27.

136. ———, *Stochastic algorithms in rarefied gas simulation*, Scuola Superiore di Catania, Laboratory for Complex Systems, Italy, October 29.

137. M. Wolfrum, *Asymptotic properties of the Floquet spectrum for delay differential equations with large delay*, Seminario ISC, Consiglio Nazionale delle Ricerche, Istituto dei Sistemi Complessi, Florence, Italy, April 30.

138. ———, *Delay differential equations with large delay*, Symposium "Evolution Equations, Related Topics and Applications", September 9–11, Helmholtz Zentrum München, September 9.

A.8.3 Talks for a More General Public

1. M. Ehrhardt, *Die optimale Flanke oder wie berechne ich die richtige Flugkurve?*, Käthe-Kollwitz-Oberschule, Berlin, January 12.

2. ———, *Die optimale Flanke oder wie berechne ich die richtige Flugkurve?*, Barnim-Oberschule, Berlin, February 12.

3. ———, *Die Mathematik des Klimawandels — Ein globales CO_2 -Modell*, Käthe-Kollwitz-Oberschule, Berlin, February 16.

4. ———, *Die Mathematik des Klimawandels — Ein globales CO_2 -Modell*, 14. Berliner Tag der Mathematik (14th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, April 25.

5. D. Hömberg, *Verzieh Dich (bloß nicht) — Über die Modellierung, Simulation und Optimierung der Wärmeausdehnung von Festkörpern*, MathInside — Überall ist Mathematik, Urania, Berlin, March 24.

6. R. Huth, *Keine Schlüsseltechnologien ohne Mathematik*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2009, WIAS, June 13.

7. A. Linke, *Wie Chemikalien "im Computer" reagieren*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2009, WIAS, June 13.

8. A. Mielke, *Mathematik und Photovoltaik*, Mathematik ist Zukunft, Berliner Wirtschaftsgespräche e.V./DFG Research Center Matheon, Berlin, February 17.

9. ———, *Warum sind moderne Materialien schlau?*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2009, WIAS, June 13.
10. G. Reinhardt, *Schiebe-Puzzle als Computersimulation*, 14. Berliner Tag der Mathematik (14th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, April 25.
11. C. Strauch, *Die Formel von Black-Scholes — Wunderwaffe der Finanzwelt?*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2009, WIAS, June 13.
12. K. Tabelow, *Magnet-Resonanz-Tomographie: Ein Blick in Funktionalität und Anatomie des Gehirns*, 14. Berliner Tag der Mathematik (14th Berlin Day of Mathematics), Humboldt-Universität zu Berlin, April 25.

A.8.4 Posters

1. I. Babushkin, S. Skupin, J. Herrmann, *Generation of tunable ultrabroad supercontinuum from THz to near-infrared in two-color ultrashort pulses in hollow capillaries*, IOP Conference "Nonlinear Photonics in Micro- and Nanostructures", London, UK, December 10.
2. W. Dreyer, C. Guhlke, *The coupling of diffusion and mechanics in phase field models in the context of hydrogen storage and lithium-ion batteries*, PF09 — 2nd Symposium on Phase-Field Modelling in Materials Science, Kerkrade, The Netherlands, August 30 – September 2.
3. M. Ehrhardt, J. Fuhrmann, A. Linke, *Finite volume methods for the simulation of flow cell experiments*, Workshop "New Trends in Model Coupling — Theory, Numerics & Applications" (NTMC'09), Paris, France, September 2–4.
4. A. Fiebach, J. Fuhrmann, *Numerical issues for reaction-diffusion processes in semiconductor photoresists*, Workshop "Evolution Equations, Related Topics and Applications", München, September 7–11.
5. J. Fuhrmann, A. Fiebach, A. Erdmann, P. Trefonas, *Acid diffusion effects between resists in freezing processes used for contact hole patterning*, 35th International Conference on Micro and Nano Engineering (MNE 2009), Ghent, Belgium, September 29–30.
6. K. Gärtner, J.A. Griepentrog, H. Langmach, *The van Roosbroeck system, its mathematical properties, and detector simulation examples*, 11th European Symposium on Semiconductor Detectors, Wildbad Kreuth, June 7–11.
7. H.-Chr. Kaiser, *Transient Kohn–Sham theory*, Jubiläumssymposium "Licht – Materialien – Modelle" (100 Jahre Innovation aus Adlershof), Berlin-Adlershof, September 7–8.
8. G. Kitavtsev, L. Recke, B. Wagner, *Derivation, analysis and numerics of reduced ODE models describing coarsening dynamics*, 3rd European Postgraduate Fluid Dynamics Conference, Nottingham, UK, July 13–16.
9. Th. Koprucki, *Spectral properties and band gap estimates for kp Hamiltonians for quantum wells*, International Nano-Optoelectronics Workshop (iNOW 2009), Stockholm, Sweden, and Berlin, Germany, August 2–15.
10. M. Naldzhieva, W. Dreyer, N. Bauermeister, *On a coupled free boundary problem for the crystal-melt interface in the vicinity of the triple point*, Conference "Optimization with Interfaces and Free Boundaries", Regensburg, March 23–26.
11. H. Neidhardt, *Trotter–Kato product formula for imaginary times*, International Congress of Mathematical Physics, Prague, Czech Republic, August 3–8.
12. J. Polzehl, K. Tabelow, *Structural adaptive smoothing diffusion tensor imaging data: The R-package dti*, 15th Annual Meeting of the Organization for Human Brain Mapping (HBM 2009), San Francisco, USA, June 18–22.

13. P.N. Racec, *Scattering states in cylindrical nanowire heterostructures*, International Nano-Optoelectronic Workshop (iNOW 2009), Stockholm, Sweden, and Berlin, Germany, August 2–15.

14. M. Radziunas, *Simulation of switching between stable unidirectional states in semiconductor ring lasers*, European Conference on Lasers and Electro-Optics and the XIth European Quantum Electronics Conference 2009 (CLEO®/Europe – EQEC 2009), Munich, June 14–19.

15. K. Tabelow, J. Polzehl, H.U. Voss, *Structural adaptive smoothing methods for high-resolution fMRI*, 15th Annual Meeting of the Organization for Human Brain Mapping (HBM 2009), San Francisco, USA, June 18–22.

16. V.Z. Tronciu, M. Lichtner, M. Radziunas, U. Bandelow, H. Wenzel, M. Spreemann, *Calculation of improved features of distributed-feedback tapered master-oscillator power-amplifiers*, European Conference on Lasers and Electro-Optics and the XIth European Quantum Electronics Conference 2009 (CLEO®/Europe – EQEC 2009), Munich, June 14–19.

17. A. Vladimirov, *Strong enhancement of interaction of optical pulses induced by oscillatory instability*, European Conference on Lasers and Electro-Optics and the XIth European Quantum Electronics Conference 2009 (CLEO®/Europe – EQEC 2009, Munich, June 14–19.

18. A. Wilms, E. Malic, J.-E. Kim, Th. Koprucki, A. Knorr, U. Bandelow, *Microscopic model of semiconductor QD-gain*, International Nano-Optoelectronic Workshop (iNOW 2009), Stockholm, Sweden, and Berlin, Germany, August 2–15.

A.9 Visits to other Institutions[6]

1. A. Bianchi, EURANDOM, Eindhoven, The Netherlands, February 15–28.
2. ———, Rheinische Friedrich-Wilhelms-Universität, Institut für Angewandte Mathematik, Bonn, March 29 – April 9.
3. ———, Technion — Israel Institute of Technology, William Davidson Faculty of Industrial Engineering and Management, Haifa, Israel, April 21 – May 7.
4. J. Elschner, University of Tokyo, Department of Mathematical Sciences, Japan, January 25 – February 13.
5. H. Hanke, Technische Universität Graz, Fakultät für Technische Mathematik und Technische Physik, Austria, November 17–20.
6. D. Hömberg, University of Tokyo, Department of Mathematical Sciences, Japan, February 22–27.
7. N. Kleemann, Université de Nancy I, Laboratoire de Mathématiques, Vandœuvre-lès-Nancy, France, November 30 – December 11.
8. D. Knees, Università degli Studi di Udine, Dipartimento di Matematica e Informatica, Italy, April 6–9.
9. ———, Consiglio Nazionale delle Ricerche, Istituto di Matematica Applicata e Tecnologie Informatiche (IMATI), Università di Pavia, Italy, September 8–11.
10. ———, Università degli Studi di Udine, Dipartimento di Matematica e Informatica, Italy, September 14–18.
11. ———, Technische Universität Graz, Institut für Numerische Mathematik, Austria, October 1 – December 31.
12. V. Krätschmer, Technische Universität Dortmund, Fachbereich Mathematik, September 6–11.
13. P. Krejčí, Consiglio Nazionale delle Ricerche, Istituto di Matematica Applicata e Tecnologie Informatiche (IMATI), Università di Pavia, Italy, March 16 – April 3.
14. P. Mathé, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, June 23 – July 15.
15. A. Mielke, Università di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, May 19–26.
16. H. Neidhardt, Doppler Institute for Mathematical Physics and Applied Mathematics, Czech Technical University, Prague, Czech Republic, March 16–20.
17. ———, Centre National de la Recherche Scientifique, Centre de Physique Théorique, Marseille, France, October 5–16.
18. A. Petrov, Lisbon University, Center for Mathematics and Fundamental Applications, Portugal, September 14–18.
19. J. Polzehl, University of Tromsø, Institute of Mathematics and Statistics, Norway, October 4–8.
20. ———, University of Minnesota, School of Statistics, Minneapolis, USA, October 16–26.
21. K.K. Sabelfeld, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, Russia, January 5–23.
22. G. Schmidt, University of Liverpool, Department of Mathematical Sciences, UK, October 14–23.
23. V. Spokoiny, École Nationale de la Statistique et de l’Analyse de l’Information (ENSAI), Rennes, France, January 13–16, October 2–13, November 17–20, November 25 – December 10.
24. ———, Yale University, Department of Economics, New Haven, USA, October 18–29.

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

25. J. Sprekels, Università di Pavia, Dipartimento di Matematica “F. Casorati”, Italy, September 20–25.
26. K. Tabelow, Cornell University New York, Weill Medical College, USA, June 23–27.
27. V.Z. Tronciu, University of the Balearic Islands, Institute for Cross-Disciplinary Physics and Complex Systems, Palma de Mallorca, Spain, June 24–28.
28. A.G. Vladimirov, University College Cork, Department of Applied Mathematics, Ireland, July 8–17.
29. W. Wagner, Institute for Pure and Applied Mathematics (IPAM), University of California, Los Angeles, USA, May 15–29.
30. ———, Università di Catania, Dipartimento di Matematica e Informatica, Italy, October 26–30.
31. L. Wilhelm, Centre National de la Recherche Scientifique, Centre de Physique Théorique, Marseille, France, October 10–16.
32. M. Wolfrum, Consiglio Nazionale delle Ricerche, Istituto dei Sistemi Complessi, Florence, Italy, April 22 – May 7.
33. ———, Technical University of Lodz, Faculty of Mechanical Engineering, Division of Dynamics, Poland, September 14–17.

A.10 Academic Teaching[7,8]

Winter Semester 2008/2009

1. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS.
2. D. Belomestny, W. Härdle, O. Okhrin, *Statistical Tools in Finance and Insurance* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
3. M. Ehrhardt, *Asymptotische Analysis* (lecture), Technische Universität Berlin, 2 SWS.
4. ———, *Transport in porösen Medien — Modellierung, Analysis und Numerik* (seminar), Technische Universität Berlin, 2 SWS.
5. ———, *Asymptotische Analysis* (practice), Technische Universität Berlin, 1 SWS.
6. J. Fuhrmann, *Integraltransformation und partielle Differentialgleichungen* (lecture), Technische Universität Berlin, 2 SWS.
7. A. Glitzky, *Grundlagen der Kontrolltheorie und optimalen Steuerung/BMS Advanced Course "Introduction to Control Theory and Optimal Control"* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
8. D. Hömberg, *Nichtlineare Optimierung* (lecture), Technische Universität Berlin, 4 SWS.
9. O. Klein, *Analytische Eigenschaften von Hysterese-Operatoren; Evolutionsgleichungen mit Hysterese-Operatoren* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
10. D. Knees, *Allgemeine Variationsmethoden I/BMS Advanced Course "General Variational Methods I"* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
11. M. Korzec, *Lineare Algebra für Ingenieure* (practice), Technische Universität Berlin, 4 SWS.
12. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS.
13. V. Spokoiny, W. Härdle, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
14. V. Spokoiny, M. Reiss, *Nichtparametrische Statistik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
15. H. Gajewski, J. Sprekels, F. Tröltzsch, R. Klein, Ch. Schütte, P. Deuflhard, R. Kornhuber, others, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS.
16. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
17. N. Togobytska, *Nichtlineare Optimierung* (practice), Technische Universität Berlin, 2 SWS.
18. M. Wolfrum, B. Fiedler, S. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS/Freie Universität Berlin, 2 SWS.

Summer Semester 2009

1. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS.

[7] SWS = semester periods per week
[8] Lectures by scholarship holders and guests during their stay at WIAS have been listed in front of those given by the collaborators of WIAS.

2. D. Belomestny, V. Krätschmer, R. Weron, *Statistical Tools in Finance and Insurance* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
3. M. Ehrhardt, *Numerik partieller Differentialgleichungen* (lecture), Technische Universität Berlin, 2 SWS.
4. ———, *Numerische Finanzmathematik* (seminar), Technische Universität Berlin, 2 SWS.
5. R. Henrion, W. Römisch, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
6. D. Hömberg, *Analysis I für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS.
7. D. Knees, *Allgemeine Variationsmethoden II/BMS Advanced Course "General Variational Methods II"* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
8. V. Krätschmer, *Advanced Methods in Quantitative Finance* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
9. A. Mielke, *Höhere Analysis II (Partielle Differentialgleichungen)/BMS Basic Course on Partial Differential Equations* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
10. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS.
11. V. Spokoiny, *Mathematische Statistik* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
12. V. Spokoiny, W. Härdle, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
13. 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.
14. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
15. M. Wolfrum, B. Fiedler, S. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS/Freie Universität Berlin, 2 SWS.

Winter Semester 2009/2010

1. P. Friz, *Finanzmathematik I* (lecture), Technische Universität Berlin, 4 SWS.
2. ———, *Topics in Stochastic Analysis* (seminar), Technische Universität Berlin, 2 SWS.
3. ———, *Finanzmathematik I* (practice), Technische Universität Berlin, 2 SWS.
4. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS.
5. D. Belomestny, M. Fengler, *Statistical Tools in Finance and Insurance* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
6. A. Glitzky, *Einführung in die Kontrolltheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
7. R. Henrion, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
8. R. Henrion, W. Römisch, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
9. D. Hömberg, *Analysis II für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS.
10. V. John, *Analysis II* (lecture), Freie Universität Berlin, 4 SWS.

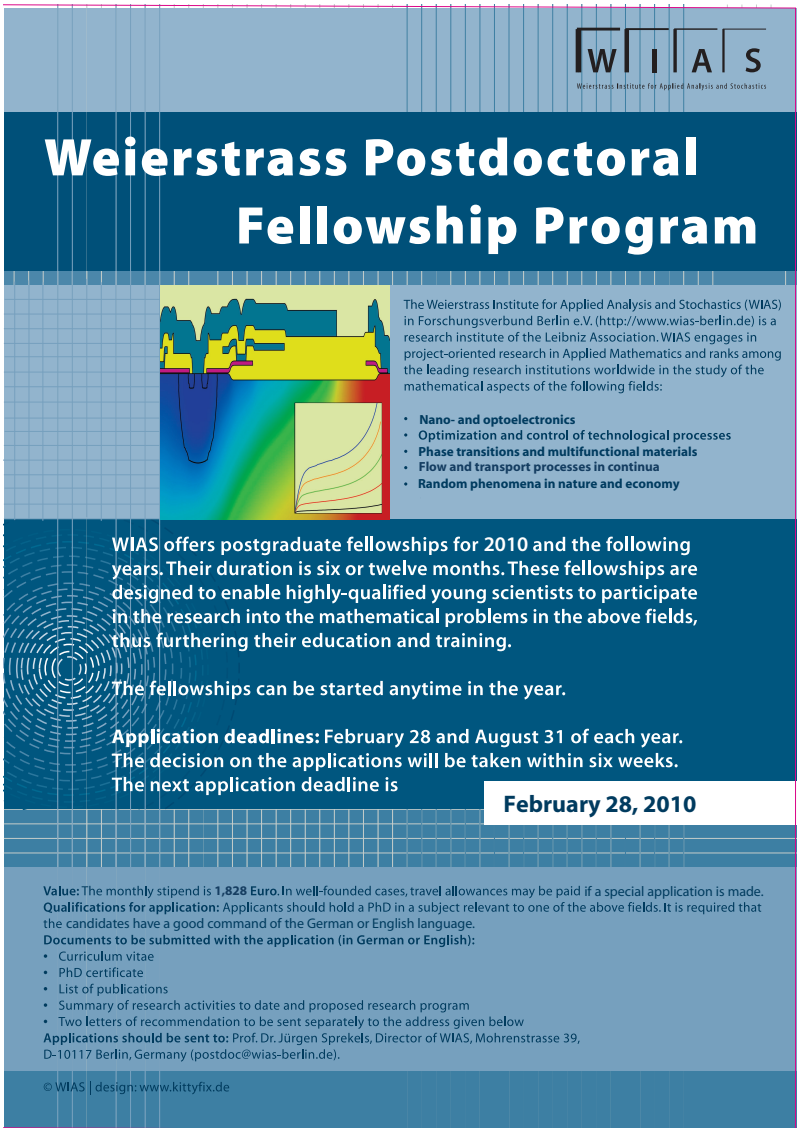
11. C. Carstensen, P. Deuflhard, H. Gajewski, V. John, R. Klein, R. Kornhuber, J. Sprekels, others, *Numerische Mathematik/Scientific Computing* (senior seminar), Freie Universität Berlin, 2 SWS.
12. D. Knees, *Partielle Differentialgleichungen II* (lecture), Technische Universität Graz, 3 SWS.
13. ———, *Variationsrechnung* (lecture), Technische Universität Graz, 2 SWS.
14. ———, *Partielle Differentialgleichungen II* (practice), Technische Universität Graz, 1 SWS.
15. ———, *Variationsrechnung* (practice), Technische Universität Graz, 1 SWS.
16. W. König, *Stochastische Modelle* (lecture), Technische Universität Berlin, 4 SWS.
17. ———, *Stochastische Modelle* (practice), Technische Universität Berlin, 2 SWS.
18. J. Blath, J. Gärtner, W. König, N. Kurt, *Stochastic Models in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
19. J.-D. Deuschel, J. Gärtner, P. Imkeller, W. König, U. Küchler, H. Föllmer, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS, 2 SWS.
20. V. Krätschmer, *Selected Topics in Banking and Insurance* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
21. M. Lichtner, *Fourieranalysis* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
22. P. Mathé, *Statistische Datenanalyse mit R* (seminar), Freie Universität Berlin, 2 SWS.
23. A. Mielke, *Variationsrechnung* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
24. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS, 2 SWS.
25. V. Spokoiny, *Nichtparametrische Verfahren* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
26. V. Spokoiny, W. Härdle, *Mathematical Statistics* (research seminar), Humboldt-Universität zu Berlin, 2 SWS.
27. J. Sprekels, *Höhere Analysis I (Funktionalanalysis)/BMS Basic Course "Functional Analysis"* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
28. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
29. M. Wolfrum, B. Fiedler, S. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS/Freie Universität Berlin, 2 SWS.

A.11 Weierstrass Postdoctoral Fellowship Program

In 2005, the Weierstrass Institute has launched the *Weierstrass Postdoctoral Fellowship Program* (see `http://www.wias-berlin.de/jobs/fellowship.jsp?lang=1`). The institute offers postgraduate fellowships with a duration of six to twelve months. These fellowships are designed to enable highly-qualified young scientists to participate in the research into the mathematical problems in the institute's main application areas 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 2009, Dr. Oleh Omel'chenko (National Academy of Sciences of Ukraine, Kiev) and Dr. Hao Wu (Fudan University, Shanghai, China) worked as fellowship holders at WIAS.



A.12 Visiting Scientists[9]

A.12.1 Guests

1. F. Abramowich, Tel Aviv University, Department of Statistics and Operations Research, School of Mathematical Sciences, Ramat Aviv, Israel, June 29 – July 6.
2. A. Aldea, National Institute of Materials Physics, Laboratory of Low Dimensional Systems, Bucharest, Romania, November 10–26.
3. P. Angot, Université de Provence, LATP, and Centre de Mathématiques et Informatique, Marseille, France, October 8–16.
4. Y. Barraud, Université de Nice Sophia-Antipolis, Laboratoire J. A. Dieudonné, France, July 12–18.
5. Ch. Besse, Université des Sciences et Technologies de Lille, Laboratoire Paul Painlevé, INRIA SIMPAF Team, France, April 5–10.
6. A.B. Bhattacherjee, University of Delhi, Atma Ram Sanatan Dharm College, India, November 16 – December 15.
7. D. Bothe, Technische Universität Darmstadt, Center for Smart Interfaces, April 26–30.
8. A. Briantais, Université Polytechnique, Centre de Mathématiques Appliquées, Palaiseau, France, April 20 – July 3.
9. O. Burylko, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, October 11–18.
10. G. Carini, Brookhaven National Laboratory, National Synchrotron Light Source, New York, USA, June 13–21.
11. K. Chełminski, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, June 29 – July 25.
12. Y. Chen, National University of Singapore, Faculty of Science, Department of Statistics and Applied Probability, October 31 – November 6.
13. R. Čiegis, Vilnius Gediminas Technical University, Department of Mathematical Modeling, Lithuania, November 1–27.
14. P. Colli, Università di Pavia, Dipartimento di Matematica, Italy, September 14–20.
15. O. Collier, École Normale Supérieure de Cachan, Département de Mathématiques Appliquées, France, May 13 – August 31.
16. P. Contucci, Università di Bologna, Dipartimento di Matematica, Italy, July 26 – August 23.
17. E. Di Stefano, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, November 7–28.
18. E. Diederichs, Freie Universität Berlin, Fachbereich Mathematik und Informatik, Institut für Mathematik, September 21 – December 18.
19. J. Dony, Free University of Brussels, Department of Mathematics, Belgium, January 19–25.
20. E. Dremkova, Halmstad University, Center for Applied Mathematics and Physics, Sweden, April 14–24.
21. M.A. Efendiev, Helmholtz Zentrum München, GmbH, Institut für Biomathematik und Biometrie, February 10–17.
22. V. Egorova, Halmstad University, Center for Applied Mathematics and Physics, Sweden, April 14–24.

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

23. I. Ermakov, Vrije Universiteit Brussel, Department of Applied Physics and Photonics, Belgium, October 26–31.
24. S.M. Ermakov, University of St. Petersburg, Faculty of Mathematics and Mechanics, Russia, November 9–22.
25. I. Esquivias, Universidad Politécnica de Madrid, Departamento de Tecnología Fotónica, Spain, November 12–15.
26. R. Eymard, Université Paris Est, Département de Mathématiques, Marne-la-Vallée, France, November 9–12.
27. K. Fokianos, University of Cyprus, Department of Mathematics and Statistics, Nikosia, February 1–5.
28. C. Giardina, Technical University of Eindhoven, Department of Mathematics and Computer Science, The Netherlands, July 26 – August 2.
29. A. Goldenshluger, University of Haifa, Department of Statistics, Israel, November 3–6.
30. L.I. Goray, Russian Academy of Sciences, Institute for Analytical Instrumentation, St. Petersburg, June 17–21.
31. S. Grönneberg, University of Oslo, Department of Mathematics, Norway, January 1–31.
32. ———, June 8–25.
33. V. Gudmundsson, University of Iceland, Science Institute, Reykjavik, May 24 – June 14.
34. N.G. Hadjiconstantinou, Massachusetts Institute of Technology, Cambridge, USA, July 5–30.
35. M. Herrmann, Oxford University, Mathematical Institute, UK, August 1–31.
36. G.C. Hsiao, University of Delaware, Department of Mathematical Sciences, Newark, USA, August 16 – September 5.
37. A. Ivanova, Halmstad University, Center for Applied Mathematics and Physics, Sweden, April 14–24.
38. E. Jarlebring, Catholic University of Leuven, Department of Computer Science, Belgium, June 8–12.
39. S. Johansen, University of Copenhagen, Department of Statistics and Operations Research, Denmark, April 27 – May 1.
40. A. Juditsky, Université Joseph Fourier, Laboratoire Jean Kuntzmann, Grenoble, France, November 3–6.
41. B. Kaltenbacher, Universität Stuttgart, Fachbereich Mathematik, February 8–12.
42. T. Kapitaniak, Technical University of Łodz, Division of Dynamics, Poland, June 7–20.
43. A. Khrabustovski, B. Verkin Institute for Low Temperature Physics and Engineering, Mathematical Department, Kharkiv, Ukraine, November 21 – December 3.
44. S. Kilianova, Comenius University, Faculty of Mathematics, Physics and Informatics, Bratislava, Slovakia, January 26–30.
45. B. Kołodziejek, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, December 7–10.
46. J. Kopfová, Silesian University in Opava, Mathematical Institute, Czech Republic, February 9–13.
47. M. Kraft, University of Cambridge, Department of Chemical Engineering, UK, September 28 – November 22.
48. K. Kuhnen, Robert Bosch GmbH, Elektrische Antriebstechnik, Systementwicklung und Simulation (CR/ARE3), Stuttgart, February 8–13.

49. F. Lanzara, Università degli Studi di Roma “La Sapienza”, Dipartimento di Matematica, Italy, January 26 – February 6.
50. ———, September 7–18.
51. J. Liu, Southeast University, Department of Mathematics, Nanjing, Republic of China, June 28 – July 20.
52. S. Lu, Austrian Academy of Sciences, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, March 30 – April 9.
53. Y. Maistrenko, Forschungszentrum Jülich, Institut für Neurowissenschaften und Medizin (INM-2), September 20 – October 20.
54. M.M. Malamud, Donetsk National University, Department of Mathematics, Ukraine, December 20–24.
55. M. Malioutov, Northeastern University, Department of Mathematics, Boston, USA, April 20 – May 14.
56. A. Maurer, München, October 19–22.
57. Ch. Meyer, Technische Universität Darmstadt, Graduate School of Computational Engineering, July 2–8.
58. A. Mezentsev, Halmstad University, Center for Applied Mathematics and Physics, Sweden, April 14–24.
59. G. Milsteyn, Ural State University, Institute of Physics and Applied Mathematics, Ekaterinburg, Russia, October 19 – December 18.
60. B. Mordukhovich, Wayne State University, Department of Mathematics, Detroit, USA, July 1–31.
61. A. Münch, University of Nottingham, School of Mathematical Sciences, UK, March 5–8.
62. ———, August 10 – September 6.
63. O. Muscato, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, August 1–8.
64. A. Nemet, ALSTOM (Switzerland) Ltd., Baden, July 13–18.
65. R. Nickl, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, May 26–29.
66. ———, September 20–26.
67. F. Nier, Université de Rennes I, Institut de Recherche Mathématique de Rennes (IRMAR), France, April 5 – May 1.
68. F. Ortegón Gallego, Universidad de Cádiz, Departamento de Matemáticas, Puerto Real, Spain, May 25–30.
69. L. Paoli, Université de Saint-Etienne, Laboratoire de Mathématiques, France, January 6 – February 6.
70. ———, June 1–14.
71. M.A. Peletier, Eindhoven University of Technology, Centre for Analysis, Scientific Computing and Applications (CASA), The Netherlands, October 14–17.
72. A. Pimenov, University College Cork, Department of Applied Mathematics, Ireland, May 19 – June 6.
73. A. Pomelnikov, Halmstad University, Center for Applied Mathematics and Physics, Sweden, April 14–24.
74. E. Presutti, Università di Roma “Tor Vergata”, Dipartimento di Matematica, Italy, November 25–28.
75. J. Rademacher, Centrum voor Wiskunde & Informatica, Department Modelling, Analysis and Simulation, Amsterdam, The Netherlands, August 10–14.
76. ———, September 14–18.

77. N. Rebrova, Tyndall National Institute at University College Cork, Photonic Device Dynamics Group, Ireland, December 10, 2008 – January 10, 2009.
78. Q. Ren, Rücker EKS GmbH, Weingarten, November 23 – December 4.
79. Y. Rinott, The Hebrew University of Jerusalem, Department of Statistics, Israel, April 13–17.
80. Y. Ritov, The Hebrew University of Jerusalem, Department of Statistics, Israel, February 17–20.
81. E. Rohan, University of West Bohemia, Faculty of Applied Sciences, Plzen, Czech Republic, October 6–16.
82. ———, October 29 – November 13.
83. R. Rossi, Università di Brescia, Dipartimento di Matematica, Italy, April 21–25.
84. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, January 20 – February 20.
85. ———, August 10 – September 9.
86. Y. Rozenholc, Université Paris Descartes, UFR de Mathématiques et d'Informatiques, France, May 15–21.
87. G. Savaré, Università di Pavia, Dipartimento di Matematica, Italy, July 8–16.
88. A. Seeger, Université d'Avignon, Département de Mathématiques, France, April 18 – May 2.
89. ———, September 13–27.
90. D. Ševčovič, Comenius University Bratislava, Faculty of Mathematics, Physics and Informatics, Slovakia, January 26–30.
91. I. Shalimova, Russian Academy of Sciences, Institute of Computational Mathematics and Mathematical Geophysics, Novosibirsk, January 28 – February 28.
92. A. Shilnikov, Georgia State University, Department of Mathematics and Statistics, Atlanta, USA, July 20–24.
93. J. Sieber, University of Portsmouth, Department of Mathematics, UK, June 7 – July 4.
94. S. Starr, University of Rochester, Department of Mathematics, USA, July 26 – August 2.
95. A. Stefanski, Technical University of Łodz, Division of Dynamics, Poland, June 7–20.
96. B. Stehlikova, Comenius University, Faculty of Mathematics, Physics and Informatics, Bratislava, Slovakia, January 26–30.
97. D. Tiba, Romanian Academy, Institute of Mathematics, Bucharest, November 30 – December 13.
98. M. Tretyakov, University of Leicester, Department of Mathematics, UK, December 4–18.
99. D. Turaev, Imperial College London, Department of Mathematics, UK, August 4–30.
100. ———, December 20–23.
101. O. Vassilieva, Halmstad University, Center for Applied Mathematics and Physics, Sweden, April 14–24.
102. M. Vinyes Raso, Polytechnic University of Catalonia, Faculty of Mathematics and Statistics, Spain, September 9 – October 8.
103. C. Visone, Università degli Studi di Napoli Federico II, Dipartimento di Ingegneria Elettrica, Naples, Italy, February 8–14.
104. M. Yamamoto, University of Tokyo, Department of Mathematical Sciences, Japan, March 8 – April 9.
105. ———, August 26 – September 1.
106. ———, September 22 – October 5.

107. B. Zaltzman, Ben Gurion University of the Negev, Jacob Blaustein Institute for Desert Research, Sede Boqer Campus, Israel, July 23–30.

108. Ch. Zanini, Università degli Studi di Udine, Dipartimento di Matematica e Informatica, Italy, July 19–24.

109. S. Zelik, University of Surrey, Faculty of Engineering and Physical Sciences, Department of Mathematics, Guildford, UK, August 19 – September 10.

110. Ch. Zheng, Brookhaven National Laboratory, National Synchrotron Light Source, New York, USA, June 8 – July 7.

A.12.2 Scholarship Holders

1. P. Friz, Technische Universität Berlin, Institut für Mathematik, WIAS, June 12, 2009 – June 11, 2014.

2. O. Omel'chenko, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, Weierstrass Postdoctoral Fellowship Program, December 1, 2008 – November 30, 2009.

3. M. Vinyes Raso, Polytechnic University of Catalonia, Faculty of Mathematics and Statistics (Mathematics), Barcelona, Spain, DAAD Fellowship, June 1 – August 31.

4. H. Wu, Fudan University, School of Mathematical Sciences, Shanghai, China, Weierstrass Postdoctoral Fellowship Program, September 1, 2008 – August 31, 2009.

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

1. M. Becker, Universität Leipzig, Research Training Group GRK 597 "Analysis, Geometry and their Interaction with the Natural Sciences", doctoral candidate, October 7, 2009 – February 28, 2010.

2. J. Giesselmann, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, doctoral candidate, since January 1.

3. O. Gloger, Technische Universität Berlin, doctoral candidate, since April 1, 2007.

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. M. Liero, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", doctoral candidate, December 1, 2008 – November 30, 2010.

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. Ch. Mukherjee, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, International Max Planck Research School "Mathematics in Sciences", doctoral candidate, October 7, 2009 – November 30, 2011.

9. L. Panizzi, Scuola Normale Superiore, Pisa, Italy, doctoral candidate, since October 1, 2008.

10. C. Patz, Humboldt-Universität zu Berlin, Institut für Mathematik, doctoral candidate, March 1, 2009 – February 28, 2010.

11. Th. Petzold, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", doctoral candidate, May 1, 2005 – December 31, 2009.

12. A. Pimenov, University College Cork, Department of Applied Mathematics, doctoral candidate, October 1, 2006 – September 28, 2009.
13. P. Schmid, Universität Leipzig, Research Training Group GRK 597 "Analysis, Geometry and their Interaction with the Natural Sciences", doctoral candidate, October 7, 2009 – February 28, 2010.
14. S. Schmidt, Universität Leipzig, Research Training Group GRK 597 "Analysis, Geometry and their Interaction with the Natural Sciences", doctoral candidate, October 7, 2009 – February 28, 2010.
15. Th. Surowiec, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", doctoral candidate, August 1, 2006 – July 31, 2009.
16. M. Thomas, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems", doctoral candidate, January 1, 2007 – December 31, 2009.

A.13 Guest Talks

1. F. Abramowich, Tel Aviv University, School of Mathematical Sciences, Ramat Aviv, Israel, *Prelude and fugue in Bayesian testimation*, July 1.
2. F. Achleitner, Universität Wien, Fakultät für Mathematik, Austria, *Bifurcation and stability of viscous shock waves in viscous conservation laws*, December 1.
3. A. Aldea, National Institute of Materials Physics, Laboratory of Low Dimensional Systems, Bucharest, Romania, *Quantum transport in mesoscopic systems: Interference and correlation effects in quantum dots*, November 18.
4. P. Angot, Université de Provence, LATP, and Centre de Mathématiques et Informatique, Marseille, France, *On the well-posed coupling between free fluid and porous flows*, October 8.
5. S. Arlot, École Normale Supérieure, Département d'Informatique, Paris, France, *Data-driven penalties for model selection*, April 22.
6. Y. Barraud, Université de Nice Sophia-Antipolis, Laboratoire J. A. Dieudonné, France, *Gaussian model selection with an unknown variance*, July 15.
7. B. Benesova, Charles University, Mathematical Institute, Prague, Czech Republic, *Shape-memory alloys subject to hard loads — Theoretical and computational issues*, February 24.
8. Ch. Besse, Université des Sciences et Technologies de Lille, Laboratoire Paul Painlevé, INRIA SIMPAF Team, France, *Open boundary conditions and computational schemes for Schrödinger equations with general potentials and nonlinearities*, April 8.
9. A.B. Bhattacherjee, University of Delhi, Atma Ram Sanatan Dharm College, India, *Cavity quantum optomechanics of ultracold atoms*, November 26.
10. G. Blanchard, Fraunhofer FIRST (IDA), Berlin, *Some results on resampling in high dimension from a non-asymptotic point of view*, January 7.
11. D. Bothe, Technische Universität Darmstadt, Center for Smart Interfaces, *Modelling and analysis of transport processes at fluidic interfaces*, April 27.
12. ———, *Nonlinear evolution equations with applications to reaction-diffusion systems*, April 29.
13. O. Burylko, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, *Bifurcations in generalization of Kuramoto–Sakaguchi model of coupled phase oscillators*, October 12.
14. A. Caiazzo, Institut National de Recherche en Informatique et en Automatique (INRIA), REO project, France, *Complex automata models for in-stent restenosis and FE schemes for blood flows in stented aneurysms*, November 23.
15. G. Carini, Brookhaven National Laboratory, National Synchrotron Light Source, New York, USA, *Photon science at Brookhaven National Laboratory: Light sources, detectors and applications*, June 18.
16. K. Chełminski, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, *On strain gradient plasticity. Modeling and global existence in the infinitesimal rate-independent case*, July 14.
17. R. Čiegis, Vilnius Gediminas Technical University, Department of Mathematical Modeling, Lithuania, *Parallel numerical algorithms for parabolic problems on graphs*, November 26.
18. P. Contucci, Università di Bologna, Dipartimento di Matematica, Italy, *Spin glass correlation inequalities: Classical and quantum*, August 12.
19. M. Dahlem, Technische Universität Berlin, Institut für Theoretische Physik, *Modeling dynamics in large scale neural populations*, June 9.

20. E. Diederichs, Freie Universität Berlin, Institut für Mathematik, *Sparse non-Gaussian component analysis with applications to conformation dynamics of biomolecular systems*, June 29.
21. P. Dondl, Universität Bonn, Hausdorff-Zentrum für Mathematik, *Pinning and depinning of nearly flat martensitic interfaces in a heterogeneous environment*, June 24.
22. J. Dony, Free University of Brussels, Department of Mathematics, Belgium, *An empirical process approach to uniform in bandwidth consistency of kernel-type estimators*, January 21.
23. P. Doukhan, Université Cergy Pontoise, Département de Mathématiques, France, *Weak dependence and some applications*, December 9.
24. V. Dymkou, Coventry University, Applied Mathematics Research Centre, UK, *MHD turbulence and spectral methods: Simulation, stabilization and control*, November 23.
25. M.A. Efendiev, Helmholtz Zentrum München, Institut für Biomathematik und Biometrie, *On a new class of degenerate parabolic systems arising in the modelling of biofilms*, February 12.
26. I. Ermakov, Vrije Universiteit Brussel, Department of Applied Physics and Photonics, Belgium, *Nonlinear dynamics of semiconductor FP and ring lasers with external optical feedback*, October 29.
27. I. Esquivias, Universidad Politécnica de Madrid, Departamento de Tecnología Fotónica, Spain, *Simulation and design of high brightness tapered lasers*, November 12.
28. R. Eymard, Université Paris Est, Département de Mathématiques, Marne-la-Vallée, France, *Application of discrete functional analysis to the convergence study of a finite volume scheme for nonlinear elliptic/parabolic problems*, November 11.
29. K. Fokianos, University of Cyprus, Department of Mathematics and Statistics, Nikosia, *On Poisson autoregression*, February 4.
30. M. Gerdts, Universität Würzburg, Institut für Mathematik, *Optimale Steuerung von Robotern*, June 16.
31. V. Gudmundsson, University of Iceland, Science Institute, Reykjavik, Iceland, *Time-dependent transport in quantum wires*, May 27.
32. M.H. Gutknecht, Eidgenössische Technische Hochschule Zürich and Technische Universität Berlin, *IDR in variations*, January 12.
33. N.G. Hadjiconstantinou, Massachusetts Institute of Technology, Cambridge, USA, *On efficient stochastic methods for solving the Boltzmann transport equation*, July 22.
34. Ch. Heinemann, Humboldt-Universität zu Berlin, Institut für Mathematik, *Homogenisierung von nichtlinearen Schrödingergleichungen*, May 27.
35. J. Hell, Freie Universität Berlin, Institut für Mathematik, *Conley index at infinity*, January 20.
36. E. Hoarau, Université Blaise Pascal, Clermont-Ferrand, France, *Finite-volume simulation of carbon steel corrosion in a nuclear waste deep repository*, November 19.
37. G.C. Hsiao, University of Delaware, Department of Mathematical Sciences, Newark, USA, *An interaction problem for the elastic body in electromagnetic field*, August 31.
38. J. Huang, Institut National de Recherche en Informatique et en Automatique (INRIA), Sophia Antipolis, France, *The Berry–Esseen theorem for normalized martingales and stochastic algorithms and applications in stochastic control*, December 23.
39. E. Jarlebring, Catholic University of Leuven, Department of Computer Science, Belgium, *Numerical methods for the spectrum of delay-differential equations*, June 11.
40. A. Jechow, Universität Potsdam, Arbeitsgruppe Photonik, *Investigation of external cavity enhanced stripe array broad area diode lasers*, April 23.

41. S. Johansen, University of Copenhagen, Institute of Mathematical Sciences, Department of Statistics and Operations Research, Denmark, *An analysis of the indicator saturation estimator as a robust regression estimator*, April 29.
42. B. Kaltenbacher, Universität Stuttgart, Institut für Stochastik und Anwendungen, *Some hysteresis models in piezoelectricity*, February 10.
43. I. Kanter, Bar-Ilan University, Physics Department, Ramat Gan, Israel, *Chaotic lasers: Synchronization, communication and ulta-fast random number generators*, June 25.
44. O. Kastner, Ruhr-Universität Bochum, Institut für Werkstoffe, *Principle investigation on the dynamics of martensitic transformations in 2D Lennard–Jones lattices*, November 24.
45. B. Kawohl, Universität Köln, Mathematisches Institut, *Overdetermined boundary value problems for the p-Laplacian*, January 7.
46. B. Khoromskij, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Tensor-structured numerical methods in high dimensional applications*, November 26.
47. A. Khrabustovski, B. Verkin Institute for Low Temperature Physics and Engineering, Mathematical Department, Kharkiv, Ukraine, *Analysis of a general linear reaction-diffusion system by means of homogenization methods*, November 26.
48. S.-J. Kimmerle, Humboldt-Universität zu Berlin, Institut für Mathematik, *Homogenization of sharp-interface models for precipitation in crystalline GaAs including mechanical stresses*, November 25.
49. C. Klapproth, Konrad-Zuse-Zentrum für Informationstechnik Berlin, *Auf dem Weg zur adaptiven numerischen Integration von dynamischen Kontaktproblemen*, May 5.
50. B. Kołodziejek, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, *On some thermomechanical model of phase transitions in steel*, December 10.
51. E. Korotyaev, Cardiff University, School of Mathematics, UK, *1D Schrödinger operator with periodic plus compactly supported potentials*, July 1.
52. M. Kraft, University of Cambridge, Department of Chemical Engineering, UK, *A moment and stochastic field method for turbulent reactive flow*, November 4.
53. K. Kuhnen, Robert Bosch GmbH, Elektrische Antriebstechnik, Systementwicklung und Simulation, Stuttgart, *Design selbstoptimierender Steuerungen*, February 10.
54. J.N. Kutz, University of Washington, Department of Applied Mathematics, Seattle, USA, *Models for high-power pulsed lasers*, June 18.
55. F. Lanzara, Università degli Studi di Roma “La Sapienza”, Dipartimento di Matematica, Italy, *Tensor product approximations of high dimensional potentials*, September 15.
56. R. Lauterbach, Universität Hamburg, Department Mathematik, *Bifurcation in homogeneous networks: Linear theory*, June 16.
57. E. Le Pennec, Université Paris Diderot, Laboratoire de Probabilités et Modèles Aléatoires, France, *Adaptive Dantzig density estimation*, October 28.
58. U. Leonhardt, University of St. Andrews, Chair in Theoretical Physics, UK, *Geometry, light and a wee bit of magic*, May 25.
59. J. Liu, Southeast University, Department of Mathematics, Nanjing, Republic of China, *Detecting the obstacles by acoustic scattering waves using singular sources*, June 30.
60. R. Loeffen, Austrian Academy of Sciences, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, *Controlled spectrally negative Lévy processes with applications*, July 14.

61. Th. Lorenz, Johann Wolfgang Goethe-Universität Frankfurt am Main, Fachbereich 12: Informatik und Mathematik, *Mutational analysis — The Cauchy problem in and beyond vector spaces*, July 7.

62. Y. Maistrenko, Forschungszentrum Jülich, Institut für Neurowissenschaften und Medizin (INM-2), *Can multistability help in desynchronizing pathologic neuronal synchrony?*, October 15.

63. M.M. Malamud, Donetsk National University, Department of Mathematics, Ukraine, *1-D Schrödinger operators with local interactions on a discrete set*, December 21.

64. M. Malioutov, Northeastern University, Department of Mathematics, Boston, USA, *On the capacity of sparse identification under linear programming analysis*, May 13.

65. A. Maurer, München, *Similarity and transfer learning*, October 21.

66. D. Meidner, Technische Universität München, Zentrum Mathematik, *Adaptive Finite-Elemente-Methoden in Ort und Zeit für Optimierungsprobleme mit Beschränkungen durch nichtlineare parabolische PDEs*, May 19.

67. D. Meschede, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Angewandte Physik, *Playing quantum marbles, or can we make individual atoms interfere with each other?*, July 2.

68. Ch. Meyer, Technische Universität Darmstadt, Graduate School of Computational Engineering, *Optimal control of static plasticity — Existence, regularization, and B-stationarity*, July 7.

69. G. Milshteyn, Ural State University, Institute of Physics and Applied Mathematics, Ekaterinburg, Russia, *Solving parabolic stochastic partial differential equations via averaging over characteristics*, December 8.

70. C. Mirasso, Universitat de les Illes Baleares, Instituto de Física Interdisciplinar y Sistemas Complejos, Palma de Mallorca, Spain, *Zero-lag synchronization: From lasers to neurons*, May 28.

71. B. Mordukhovich, Wayne State University, Department of Mathematics, Detroit, USA, *Some new developments and applications of variational analysis*, July 13.

72. R. Müller, Humboldt-Universität zu Berlin, Institut für Mathematik, *Finite element approximation of phase field models: Error control past topological changes*, March 9.

73. D. Neher, Universität Potsdam, Institut für Physik und Astronomie, *Structuring polymer layers for (opto)electronic applications*, March 2.

74. A. Nemet, ALSTOM (Switzerland) Ltd., Baden, *Gas turbines for efficient, flexible and clean power generation — How ALPEG/BOP supports mastering the challenges in development*, July 16.

75. R. Nickl, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, *Confidence bands in density estimation*, May 27.

76. ———, *Adaptive density estimation, smoothed empirical measures and the Kiefer–Wolfowitz theory revisited*, September 22.

77. F. Nier, Université de Rennes I, Institut de Recherche Mathématique de Rennes (IRMAR), France, *Return to the equilibrium and pseudospectral estimates: A toy model*, April 15.

78. O. Omel'chenko, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, Ukraine, *Synchronization modes in nonlocally coupled phase oscillators*, June 29.

79. ———, *Dynamics of chimera states*, October 12.

80. F. Ortegón Gallego, Universidad de Cádiz, Departamento de Matemáticas, Puerto Real, Spain, *Analysis of an induction-conduction model with degenerate electric conductivity*, May 26.

81. L. Paoli, Université de Saint-Etienne, Laboratoire de Mathématiques, France, *A velocity-based time-stepping scheme for vibro-impact problems*, January 21.

82. M.A. Peletier, Eindhoven University of Technology, Centre for Analysis, Scientific Computing and Applications (CASA), The Netherlands, *Unification of diffusion and reaction as a Wasserstein gradient flow*, October 16.

83. A. Pikovsky, Universität Potsdam, Institut für Physik und Astronomie, *Hierarchical populations of coupled oscillators: Nonlinear coupling and partial integrability*, October 12.

84. S.Y. Pilyugin, St. Petersburg State University, Faculty of Mathematics and Mechanics, Russia, *Structural stability of diffeomorphisms and shadowing properties*, November 3.

85. E. Presutti, Università di Roma "Tor Vergata", Dipartimento di Matematica, Italy, *Phase transitions in the continuum: Results and open problems*, November 27.

86. J. Rademacher, Centrum Wiskunde & Informatica Amsterdam, The Netherlands, *Lyapunov–Schmidt reduction for unfolding heteroclinic networks of equilibria and periodic orbits with tangencies*, January 27.

87. Y. Rinott, The Hebrew University of Jerusalem, Department of Statistics, Israel, *Gladiators games, statistical games, and inequalities*, April 15.

88. M. Röger, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Perturbed Allen–Cahn equation and forced mean curvature flow*, January 26.

89. E. Rohan, University of West Bohemia, Faculty of Applied Sciences, Plzen, Czech Republic, *On homogenization of a fluid saturated medium with dual porosity (application to the bone modeling)*, November 4.

90. A. Rösch, Universität Duisburg-Essen, Fachbereich Mathematik, *Discretization concepts for optimal control problems*, November 5.

91. R. Rossi, Università di Brescia, Dipartimento di Matematica, Italy, *Interplay of viscosity and dry friction in rate-independent evolutions with nonconvex energies*, April 22.

92. L. Rossovskii, Peoples' Friendship University of Russia, Moscow, *Boundary-value problems connected with the pantograph equation and their elliptic analogs*, May 26.

93. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, *Delamination problems*, February 4.

94. Y. Rozenholc, Université Paris Descartes, UFR de Mathématiques et d'Informatiques, France, *Denoising dynamical image : Application to angiogenesis evaluation using DCE-CT*, May 20.

95. E. Salje, Cambridge University, Department of Earth Sciences, UK, *Microstructures in ferroelastics*, May 27.

96. O. Sander, Freie Universität Berlin, Institut für Mathematik, *Kontaktprobleme, und wie man sie mit Dune elegant lösen kann*, October 15.

97. G. Savaré, Università di Pavia, Dipartimento di Matematica, Italy, *A variational approach to gradient flows in metric-measure spaces*, July 15.

98. M. Schienle, Humboldt-Universität zu Berlin, Institut für Statistik und Ökonometrie, *Nonparametric nonstationary regression*, January 14.

99. A. Schlömerkemper, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *On a discrete-to-continuum model for cracks*, January 7.

100. R. Schneider, Technische Universität Berlin, Institut für Mathematik, *Size consistent solution of the electronic Schrödinger equation*, August 31.

101. A. Schuppert, Bayer Technology Services GmbH/Aachen Institute for Advanced Study in Computational Engineering Science (AICES) — the Graduate School of the RWTH, *Modelling of interactome networks for drug development and personalized medicine*, March 3.

102. F. Schuricht, Technische Universität Dresden, Institut für Analysis, *The eigenvalue problem for the 1-Laplace operator*, January 14.

103. A. Seeger, Université d'Avignon, Département de Mathématiques, France, *Eigenvalue analysis of linear complementarity systems*, April 28.

104. ———, *Variational and geometric analysis of convex cones: Old and new results*, September 22.

105. D. Ševčovič, Comenius University Bratislava, Faculty of Mathematics, Physics and Informatics, Slovakia, *Higher order estimates for the curvature and nonlinear stability of stationary solutions for curvature flow with triple junction*, January 28.

106. A. Shilnikov, Georgia State University, Department of Mathematics and Statistics, Atlanta, USA, *Multistability in models of center pattern generators*, July 21.

107. J. Sieber, University of Portsmouth, Department of Mathematics, UK, *Using feedback control to find unstable phenomena in experiments*, June 11.

108. ———, *Floquet spectra for DDEs with large delay*, July 2.

109. O. Sigmund, Technical University of Denmark, Department of Mechanical Engineering, Lyngby, *Topology optimization and its applications to mechanics and wave propagation problems*, May 25.

110. A.L. Skubachevskii, Moscow State Aviation Institute, Russia, *Elliptic functional differential equations with degeneration*, February 10.

111. P.E. Stelzig, Technische Universität München, Zentrum Mathematik, Garching, *Homogenization of certain laminated many-body structures under global noninterpenetration constraints*, July 8.

112. T. Stoica, Forschungszentrum Jülich, Institut für Bio- and Nanosysteme, *Surface-induced phenomena in GaN and InN nanowires*, March 4.

113. B. Suhr, Universität Bremen, Zentrum für Technomathematik, *Modellierung und FE-Simulationen von Verzugsverhalten bei Stahl*, February 17.

114. B. Tarigan, Bandung Institute of Technology, Department of Mathematics, Indonesia, *Fast rates of convergence for adaptive classification*, June 2.

115. D. Tiba, Romanian Academy, Institute of Mathematics, Bucharest, *Finite element approximation in shape optimization problems with Neumann or mixed boundary conditions*, December 8.

116. L. Tuckermann, École Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Laboratoire de Physique et Mécanique des Milieux Hétérogènes, France, *Turbulent-laminar patterns in plane Couette flow*, November 10.

117. D. Turaev, Imperial College London, Department of Mathematics, UK, *On stickiness and flicker-noise*, August 11.

118. ———, *A Fermi acceleration machine*, December 22.

119. S. Ulbrich, Technische Universität Darmstadt, Fachbereich Mathematik, *Adaptive Multilevel-Verfahren für die Optimierung mit partiellen Differentialgleichungen*, June 9.

120. H. van Zanten, Eindhoven University of Technology, Department of Mathematics and Computer Science, The Netherlands, *Nonparametric Bayesian inference for discretely observed diffusions*, June 10.

121. M. Vinyes Raso, Polytechnic University of Catalonia, Faculty of Mathematics and Statistics, *Single index classification*, September 29.

122. C. Visone, Università degli Studi di Napoli Federico II, Dipartimento di Ingegneria Elettrica, Naples, Italy, *Hysteresis in magnetostrictive devices: Application to smart sensors and actuators*, February 10.

123. M. Wagner, Brandenburgische Technische Universität Cottbus, Mathematisches Institut, *Generalized convexity notions in optimal control problems from image processing*, January 21.

124. K. Weichert, Max-Planck-Institut für Festkörperforschung Stuttgart, *LiFePO4 defect chemistry and phase transition to FePO4*, April 27.

125. B. Witzigmann, Universität Kassel, Fachgebiet Computational Electronics and Photonics, *Computational modeling of semiconductor nanostructures for optoelectronics*, October 26.

126. M. Yamamoto, University of Tokyo, Department of Mathematical Sciences, Japan, *Uniqueness by the two dimensional local Dirichlet-to-Neumann map on an arbitrary subboundary*, March 26.

127. ———, *Uniqueness and stability results in shape determination*, August 31.

128. B. Zaltzman, Ben Gurion University of the Negev, Jacob Blaustein Institute for Desert Research, Sede Boqer Campus, Israel, *Probing the extended space charge by harmonic disturbances*, July 27.

129. S. Zelik, University of Surrey, Department of Mathematics, Guildford, UK, *Quasi-linear strongly damped wave equations: Well-posedness and attractors*, September 1.

130. Ch. Zheng, National Synchrotron Light Source, Brookhaven National Laboratory, New York, USA, *Gaussian beam method for the boundary value problem of Helmholtz equation in the high frequency regime*, July 1.

131. N. Zhuravlev, Peoples' Friendship University of Russia, Moscow, *Methoden zur qualitativen Untersuchung periodischer Lösungen von Funktionaldifferentialgleichungen*, November 24.

A.14 Software

adimpro (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: karsten.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 of 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: joerg.polzehl@wias-berlin.de)

AWS is a contributed package within the R-Project for Statistical Computing containing a reference implementation of the adaptive weights smoothing algorithms for local constant likelihood and local polynomial regression models. Binaries for several operating systems are available from the Comprehensive R Archive Network (http://cran.r-project.org).

AWS for AMIRA (TM) (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: karsten.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/).

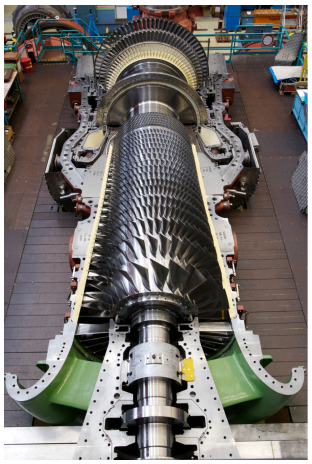


Fig. 1: *©2009 Bryon Paul McCartney www.image-engineers.com all rights reserved*

Assembly of an Alstom GT26 gas turbine at the Mannheim, Germany, facility

BOP (contact: J. Borchardt, phone: +49 30/20372-485, e-mail: juergen.borchardt@wias-berlin.de)

The **B**lock **O**riented **P**rocess simulator BOP 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: hans-joachim.mucha@wias-berlin.de)

The statistical software ClusCorr98® performs exploratory data analysis with the focus on cluster analysis, classification, and multivariate visualization. A highlight is the pairwise data clustering for finding groups in data. Another highlight is the automatic validation technique of cluster analysis results performed by a general built-in validation tool based on resampling techniques. It can be considered as a three-level assessment of stability. The first and most general level is decision-making regarding the appropriate number of clusters. The decision is based on well-known measures of correspondence between partitions. Second, the stability of

each individual cluster is assessed based on measures of similarity between sets. It makes sense to investigate the (often quite different) specific stability of clusters. In the third and most detailed level of validation, the reliability of the cluster membership of each individual observation can be assessed.

ClusCorr98® runs in the host application Excel 2007. Hence it makes use of the new "Big Grid" spreadsheets.

Further information: http://www.wias-berlin.de/software/ClusCorr98

DiPoG (contact: A. Rathsfeld, phone: +49 30/20372-457, e-mail: andreas.rathsfeld@wias-berlin.de)

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

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

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

dti (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: karsten.tabelow@wias-berlin.de)

dti is a contributed package within the R-Project for Statistical Computing. The package contains tools for the analysis of diffusion-weighted magnetic resonance imaging data (DWI) in the context of the diffusion tensor (DTI) model. It can be used to read DWI data, to estimate the diffusion tensor, for adaptive smoothing of DWIs, and for two- and three-dimensional visualization of the results. The package is available from the Comprehensive R Archive Network (http://cran.r-project.org).

EDR (contact: J. Polzehl, phone: +49 30/20372-481, e-mail: joerg.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).

fmri (contact: K. Tabelow, phone: +49 30/20372-564, e-mail: karsten.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).

gltools (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.fuhrmann@wias-berlin.de)

gltools is a library for the visualization of finite volume and finite element computations on unstructured triangular and tetrahedral meshes. Unlike many other packages, it has been designed in such a way that it can be integrated into the numerical solution process. Therefore, the software package can be used not only for the support of pre- and postprocessing, but also for debugging during the development of numerical algorithms. In particular, gltools can be used as an integral part of the toolbox pdelib. Using the OpenGL API 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 more information under http://www.wias-berlin.de/software/gltools.

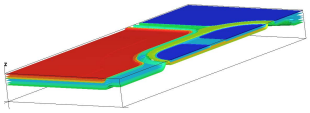


Fig. 2: *gltools visualization of a logarithmic representation of the doping in a 3D DEPFET device discretized with* $3 \cdot 10^6$ *points*

LDSL-tool (contact: M. Radziunas, phone: +49 30/20372-441, e-mail: mindaugas.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 multisection semiconductor lasers and different coupled laser devices. This software is used to investigate and 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`

MooNMD (contact: V. John, phone: +49 30/20372-561, e-mail: volker.john@wias-berlin.de)

`MooNMD` is a flexible finite element package for the solution of steady-state and time-dependent convection-diffusion-reaction equations, incompressible Navier–Stokes equations, and coupled systems consisting of these types of equations, such as population balance systems. Important features of `MooNMD` are

- the availability of more than 100 finite elements in one, two, and three space dimensions (conforming, nonconforming, discontinuous, higher-order, isoparametric, with bubbles),
- the use of implicit time-stepping schemes (θ-schemes, DIRK schemes, Rosenbrock–Wanner schemes),
- the application of a multiple-discretization multi-level (MDML) preconditioner in Krylov subspace methods.

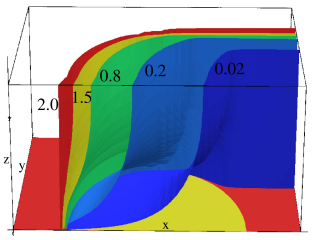


Fig. 3: *Concentration isosurfaces in a thin layer flow cell*

pdelib (contact: J. Fuhrmann, phone: +49 30/20372-560, e-mail: juergen.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, which is part of the package.

Please see also `http://www.wias-berlin.de/software/pdelib`.

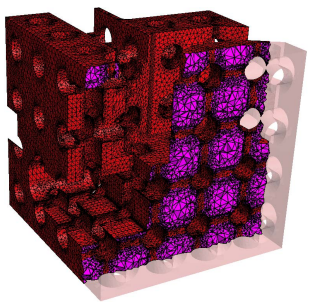


Fig. 4: *A cut view of a constrained Delaunay tetrahedral mesh of a complex 3D solid generated by* `TetGen`

TetGen (contact: H. Si, phone: +49 30/20372-446, e-mail: hang.si@wias-berlin.de)

`TetGen` is a mesh generator for three-dimensional simplex meshes as they are used in finite volume and finite element computations. It generates the Delaunay tetrahedralization, Voronoi diagram, and convex hull for three-dimensional point sets. For three-dimensional domains with piecewise linear boundary, it constructs constrained Delaunay tetrahedralizations and quality tetrahedral meshes. Furthermore, it is able to create boundary-conforming Delaunay meshes in a number of cases including all polygonal domains with input angles larger than 70°.

More information is available at `http://www.tetgen.org`.

WIAS-3dReduce (contact: I. Bremer, phone: +49 30/20372-315, e-mail: ingo.bremer@wias-berlin.de)

Based on SGI's OpenGL Performer and COG, this is a software for optimizing the visualization performance of three-dimensional objects in a virtual reality environment. It reduces the number of surface vertices and triangles with or without changing the visible geometry. Automatic level-of-detail generation is included. Many three-dimensional formats are supported through Performer loader plugins, especially VRML, Open Inventor, and Realax.

The package is distributed under the name `rfreduce` as part of Rücker Factory Invision by Rücker EKS GmbH (holger.haemmerle@ruecker.de).

A web interface for a demo version is available on request at `http://www1.wias-berlin.de/~bremer/cgi/reduce/reduce`.

WIAS-HiTNIHS (contact: O. Klein, phone: +49 30/20372-533, e-mail: olaf.klein@wias-berlin.de)

The WIAS **Hi**gh **T**emperature **N**umerical **I**nduction **H**eating **S**imulator constitutes a transient simulation tool for the temperature evolution in axisymmetric technical systems that are subject to induction or resistance heating. The simulator accounts for heat transfer by radiation through cavities, and it allows for changes in the material parameters due to the rising temperature and for some kinds of anisotropy within the thermal conductivity. It is also possible to use `WIAS-HiTNIHS` just to compute axisymmetric magnetic scalar potentials, the resulting magnetic fields, and/or the resulting heat sources. In particular, one can compute so-called *traveling magnetic fields* and resulting Lorentz forces acting on conducting liquids.

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

Further information: `http://www.wias-berlin.de/software/hitnihs`.

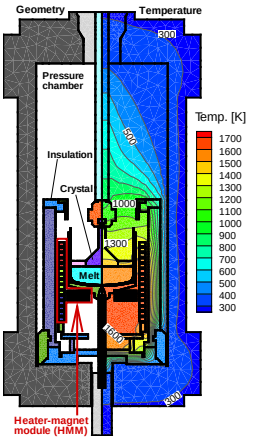


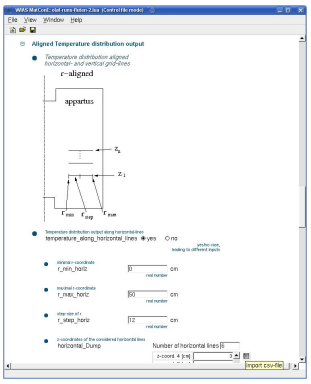
Fig. 5: *A liquid-encapsulated Czochralski (LEC) crystal growth configuration from Leibniz Institute for Crystal Growth (IKZ), with an internal heater-magnet module and a temperature distribution, computed by* `WIAS-HiTNIHS`*. The isotherms on the right-hand side are spaced at 100 K*

WIAS-MatConE (contact: O. Klein, phone: +49 30/20372-533, e-mail: olaf.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. They 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 requiring the software developer to deal with the details of GUI development.



WIAS-SHarP (contact: W. Weiss, phone: +49 30/20372-478, e-mail: wolf.weiss@wias-berlin.de)

Based on the numerical toolbox `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 base with material parameters for several 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, the numerical algorithm uses error-based time and space adaptivity.

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

WIAS-TeSCA (contact: R. Nürnberg, phone: +49 30/20372-570, e-mail: reiner.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 describing the currents of electrons and holes within the device. Thus, efficient numerical procedures for both the stationary and the transient simulation have been implemented, the spatial structure of which is a finite volume method. The underlying finite element discretization allows the simulation of arbitrarily shaped two-dimensional device structures.

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

The semiconductor device simulation package WIAS–TeSCA operates in a Linux environment on desktop computers.

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

WIAS-QW (contact: Th. Koprucki, phone: +49 30/20372-508, e-mail: thomas.koprucki@wias-berlin.de)

WIAS–QW is a numerical code for the simulation of strained multi-quantum-well structures. Based upon multiband 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 performed self-consistently, 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.