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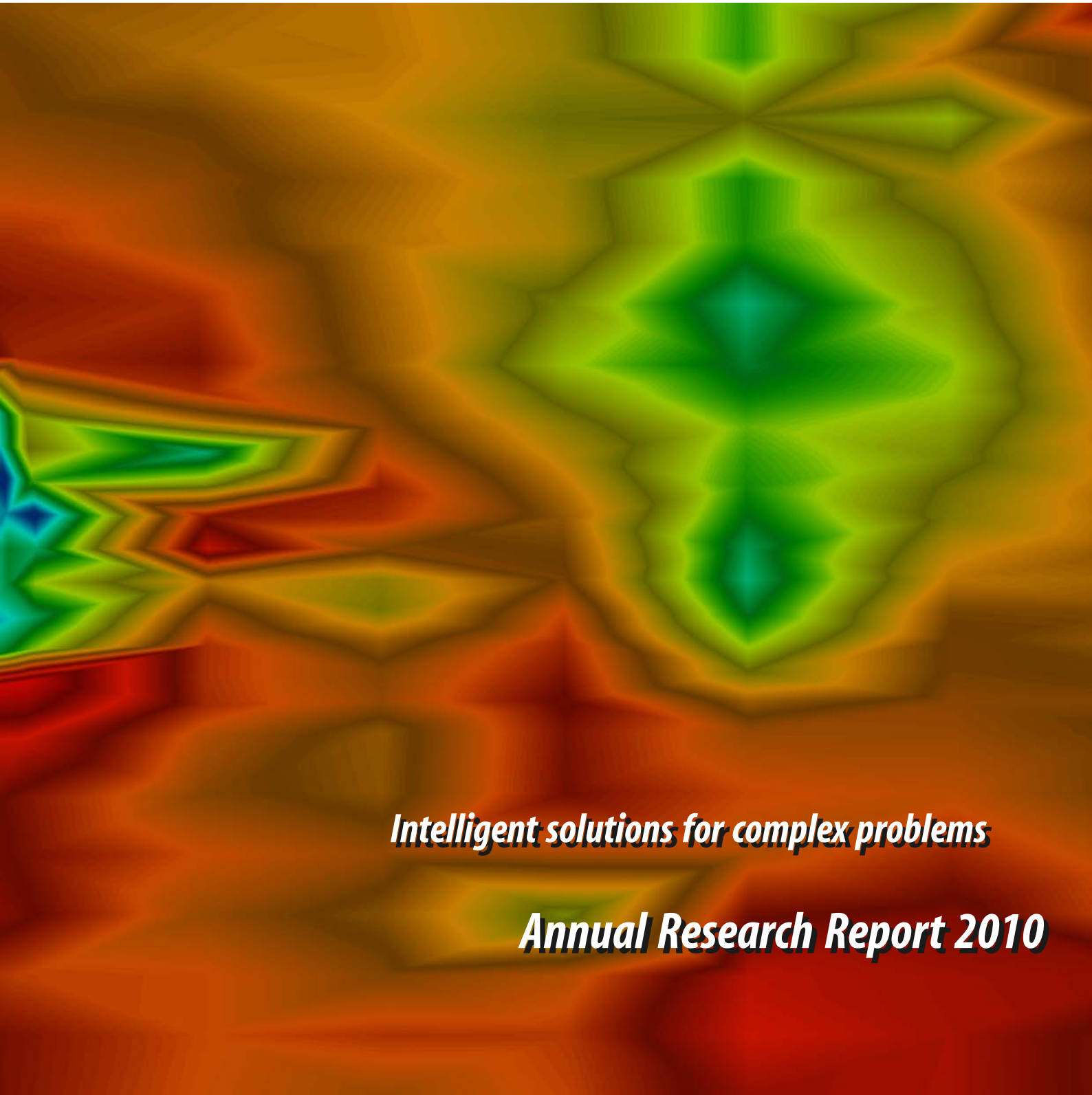
Weierstrass Institute for Applied Analysis and Stochastics



Intelligent solutions for complex problems

Annual Research Report 2010

Cover figure: Simulation of a turbulent wind tunnel experiment

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The Weierstrass Institute for Applied Analysis and Stochastics, Leibniz Institute in Forschungsverbund Berlin e.V. (WIAS, member of the Leibniz Association), presents its Annual Report 2010. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2010. Following a more general introduction in part one, in its second part eight 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 2010 was marked by two extraordinary successes for WIAS. In early July, the institute's evaluation by the Senate of the Leibniz Association, which is due every seven years, took place. The resulting judgement of the evaluation panel was so extremely positive that we can only be proud; we will have to work hard in the upcoming years to meet the expectations expressed by it. As a consequence, the joint financing of WIAS by the Federal Government of Germany and the German Länder will continue for another seven years.

An extraordinary event, a real breakthrough for the institute's international reputation, was a decision taken by the General Assembly of the International Mathematical Union (IMU) in Bangalore (India) on August 16: in the competition for hosting the future Permanent IMU Secretariat, the General Assembly voted for the WIAS offer. As a consequence of this decision, the Weierstrass Institute became, starting from January 2011, the official address of the IMU.

All this happened under very strong international competition and was only possible with the generous financial support provided by the Federal Ministry of Education and Research (BMBF) and the Berlin Senate Department for Education, Science and Research; WIAS gratefully acknowledges that these two governmental institutions agreed to support the Permanent IMU Office financially at equal parts. We also have to thank the entire mathematical community of Berlin and the German Mathematical Society (DMV) for their enthusiastic support of the WIAS application; also several other funding agencies such as the German Research Foundation (DFG), the Alexander von Humboldt Foundation (AvH), the Deutsche Telekom Foundation, the Einstein Foundation Berlin, and the Stifterverband für die Deutsche Wissenschaft (a German industry initiative promoting science and learning) made important contributions to the WIAS bid.

Besides these two all-important events of the year 2010, WIAS continued its scientific work, further consolidating 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: altogether, 48 additional co-workers could be financed from grants, the largest number ever.

Of particular scientific importance in the acquisition of grants was the ERC Advanced Grant won by the deputy director of WIAS, Prof. Dr. Alexander Mielke. His work at the institute will be supported for five years by a total of 1.4 million Euros. We also congratulate Prof. Dr. Peter Friz, non-resident member of WIAS, for receiving an ERC Starting Grant in 2010. Another outstanding honor was awarded to a WIAS member: Dr. Pierre-Etienne Druet was bestowed the Nachwuchspreis (Young Scientists' Prize) 2010 of the Leibniz Association for his dissertation.

The high rank of WIAS in the mathematical community was also witnessed by the fact that the long success story of transfer of knowledge via "brains" through the institute's members continued also in 2010. Four calls for professorships were received by members of WIAS: Dr. Klaus Krumbiegel was offered a junior professorship at the University of Leipzig (which he declined), PD Dr. Barbara Wagner received a call to a temporary W2 professorship at the Technische Universität Berlin, and Dr. Denis Belomestny was offered a professorship at the University of Twente and a W3 professorship at the University of Duisburg-Essen. Since the institute's foundation in 1992, a total of 45 calls has been received by WIAS members, a truly remarkable output of which we are proud.

Ten 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 cornerstone of this cooperation is the fact that in 2010, altogether six leading members of WIAS, including the director and his deputy, held WIAS-funded special chairs at the Berlin universities.

The highlight of cooperation with the mathematical institutions in Berlin was also in 2010 the joint operation of the DFG Research Center MATHEON "Mathematics for key technologies" located at the Technische Universität Berlin. In January 2010, MATHEON was evaluated by the DFG with excellent marks. As a result, the DFG funding of MATHEON was extended for a third period until May 2014. Until then, 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 22 of its subprojects. In turn, on Dec. 31, 2010, 17 scientific collaborators and several student assistants employed at WIAS were funded by MATHEON.

Another big success story for the mathematical community of Berlin is the "Berlin Mathematical

School" (BMS), which 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).

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.

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 May 2011

J. Sprekels

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1 WIAS in 2010

- 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), *Leibniz Institute in Forschungsverbund Berlin e.V.* (Leibniz-Institut im Forschungsverbund Berlin e. V., FVB) is one of eight scientifically independent member institutes of the *Leibniz Association* forming the legal entity FVB. 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 to 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

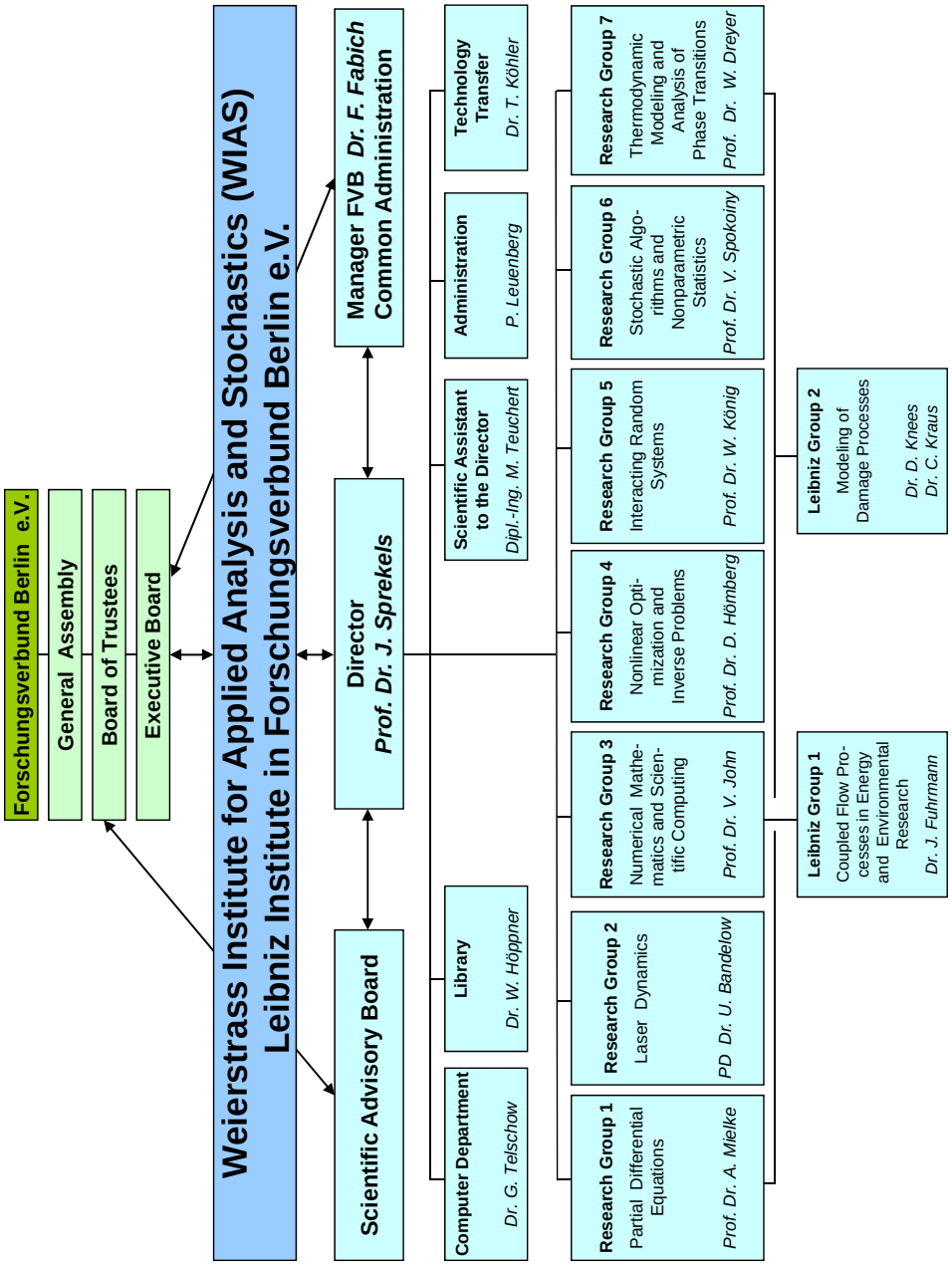
To fulfill its mission, WIAS was in 2010 organized into the departments for technical services, the seven scientific research groups, and two Leibniz groups[1]:

RG 1. Partial Differential Equations
RG 2. Laser Dynamics
RG 3. Numerical Mathematics and Scientific Computing

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

RG 4. Nonlinear Optimization and Inverse Problems
RG 5. Interacting Random Systems
RG 6. Stochastic Algorithms and Nonparametric Statistics
RG 7. Thermodynamic Modeling and Analysis of Phase Transitions
LG 1. Coupled Flow Processes in Energy and Environmental Research
LG 2. Modeling of Damage Processes

The following organization chart gives an overview of the organizational structure of WIAS in 2010:



1.2.2 Main Application Areas

The research at WIAS focused in 2010 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 three promising modern technologies:

- **Optical technologies** (in particular, diffractive and laser structures, semiconductor devices, and optical fibers)
- **Semiconductor crystal growth**
- **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 2010 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, special research topics are listed that were addressed in 2010 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 and RG 2)
- Laser structures (multisection lasers, VCSELs, quantum dots; in RG 1, RG 2, and RG 3)
- 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 continuum 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)

- Stochastic modeling of phase transitions (in RG 5)
- 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, soot; in RG 1, RG 3, RG 5, and RG 7)
- Modeling of nanostructures of thin films on crystalline surfaces (fluid films, thin film solar cells; in RG 1 and RG 7)
- Stochastic particle systems as efficient solvers of kinetic equations (in RG 5)

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 prices, 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 and statistical processes in nonhomogeneous media (in RG 5, RG 6, and RG 7)
- Stochastic description of critical phenomena (in RG 5)

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 2010, having raised a total of almost 3 million euros, from which 48 additional researchers (+ 6.5 outside WIAS; Dec. 31, 2010) have been financed. In total in 2010, 39.4 per cent of the total budget of WIAS and 47.5 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 again 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 2010, MATHEON was granted a third funding period until 2014. Annually, DFG funds exceeding 5.5 million euros flow into Berlin for MATHEON. In 2010, 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; Prof. D. Hömberg (RG 4), Scientist in Charge of the Application Area C "Production"; and WIAS members participated in the management of 22 of its subprojects. In turn, on Dec. 31, 2010, 17 scientific collaborators and several student assistants at WIAS were funded by MATHEON.

1.3.2 Graduate School *Berlin Mathematical School (BMS)*

Berlin's mathematicians won this graduate school, which is run by the three major Berlin universities, 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.

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

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 funding period runs from July 2006 to March 2011, is located at the Technische Universität Berlin.

1.3.4 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.

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

This Collaborative Research Center began its work on January 1, 2008 (first funding period: until December 2011). WIAS participates in the sub-projects "Multi-dimensional modeling and simulation of VCSEL devices" (RG 1, RG 2, and RG 3) and "Effective models, simulation and analysis of the dynamics in quantum-dot devices" (RG 2 and RG 7).

1.3.6 DFG Priority Program SPP 1164 *Nano- and Microfluidics: Bridging the Gap between Molecular Motion and Continuum Flow*

This priority program is aimed at bridging the gap between molecular motion and continuum flow by an interdisciplinary research effort from physics, engineering, chemistry, biology and medical technology. WIAS participated in the second funding period (2006–2008, principal investigators A. Muench/B. Wagner) and the third funding period (2008–2010, principal investigator Priv.-Doz. Dr. B. Wagner) with the subproject „Mathematical modeling, analysis, numerical simulation of thin films and droplets on rigid and viscoelastic substrates, emphasizing the role of slippage“ (RG 7).

1.3.7 DFG Priority Program SPP 1204 *Algorithms for Fast, Material-specific Process-chain Design and Analysis in Metal Forming*

The SPP 1204 is devoted to the development of material-oriented models and fast algorithms for the design and control of process chains in metal forming. WIAS participates in the sub-project "Simulation and control of phase transitions and mechanical properties during hot-rolling of multi-phase steel".

1.3.8 DFG Priority Program SPP 1276 *MetStröm: Multiple Scales in Fluid Mechanics and Meteorology*

Started in 2007, the project *Reference experiments in a multiphase wind tunnel, numerical simulations and validation* within SPP 1276 runs in the second funding period. Numerical methods for turbulent two-phase flows are developed and validated with experimental data, which are obtained from the collaborator within the project.

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

This unit, coordinated by the head of RG 5, Prof. W. König, and funded in its second period since 2009, continued its activities in Germany and, in particular, organized two world-class workshops in 2010 in Berlin. Research is devoted to a rigorous meso- and macroscopic analysis of large interacting systems with random input on microscopic scales.

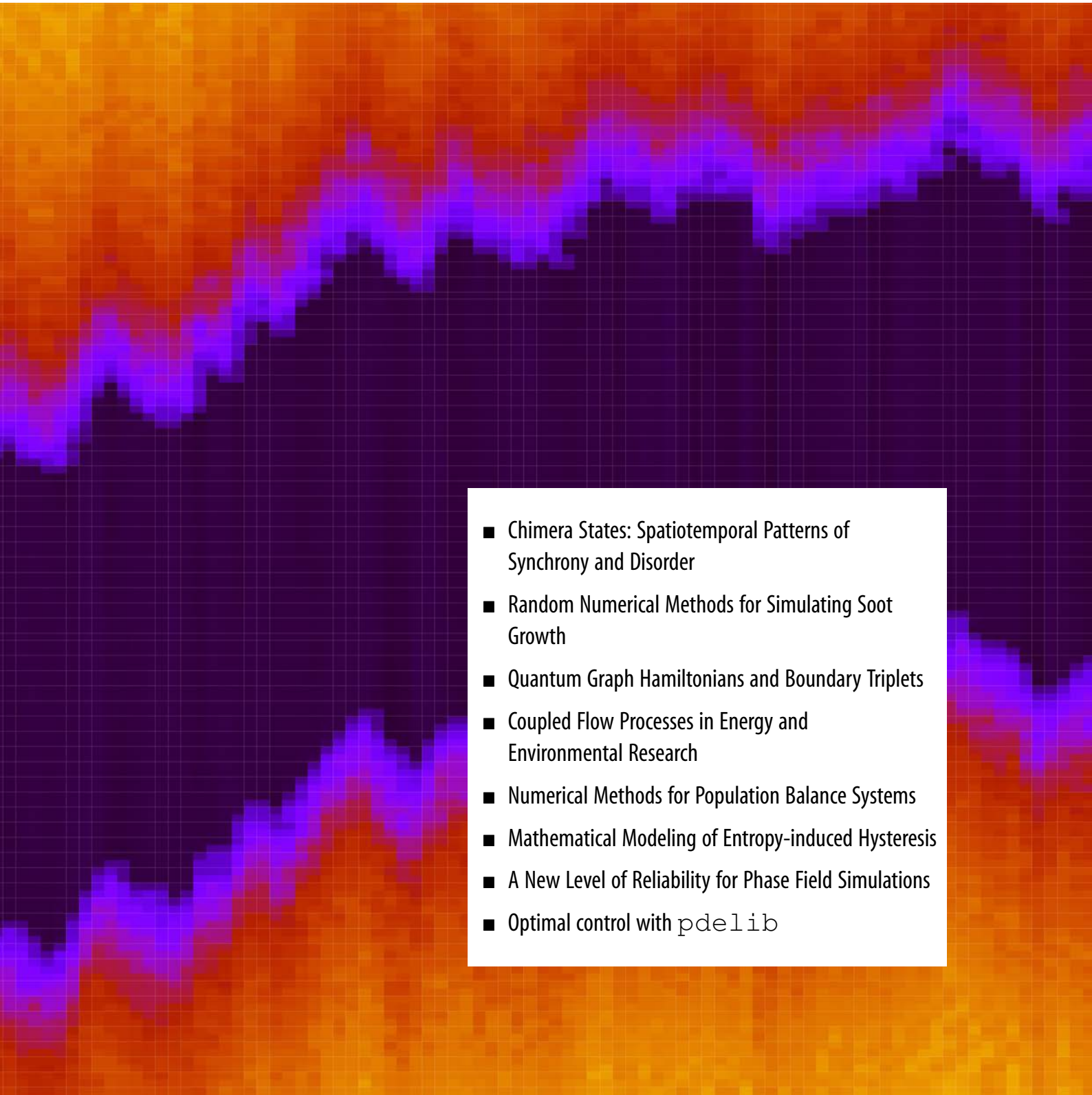
1.3.10 DFG Research Unit 797 *Analysis and Computation of Microstructure in Finite Plasticity*

WIAS participates in this research unit in the sub-project "Regularizations and relaxations of time-continuous problems in plasticity" (RG 1; second funding period: until August 2014).

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

This project started in July 2007 and ended in June 2010. 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).

2 Scientific Highlights



- Chimera States: Spatiotemporal Patterns of Synchrony and Disorder
- Random Numerical Methods for Simulating Soot Growth
- Quantum Graph Hamiltonians and Boundary Triplets
- Coupled Flow Processes in Energy and Environmental Research
- Numerical Methods for Population Balance Systems
- Mathematical Modeling of Entropy-induced Hysteresis
- A New Level of Reliability for Phase Field Simulations
- Optimal control with `pdelib`

2.1 Chimera States: Spatiotemporal Patterns of Synchrony and Disorder

Oleh Omel'chenko and Matthias Wolfrum

Fig. 1: *"Chimera of Arezzo": an Etruscan bronze statue*

According to Greek mythology, a chimera is a monstrous creature that is composed of the parts of different animals (see Figure 1). Today we use this term to characterize something consisting of incongruous parts, such that it seems impossible or hard to believe. Recently, the term "chimera state" has been introduced for newly discovered solutions in certain systems of coupled oscillators [1]. These solutions are both composed of incongruous parts and hardly believable to exist. Whereas it was known before that in such systems synchronous motion as well as an incoherent asynchronous motion are possible, nobody expected solutions composed of regions with synchronous and asynchronous motion coexisting at the same time under homogeneous conditions [3]. However, at the same time this remarkable new phenomenon of a self-organized structure could serve as a prototype for various physical effects, e.g., coexistence of synchronous and asynchronous neural activity (so-called *bump states*) or turbulent-laminar flow patterns in fluid mechanics.

From a mathematical point of view, chimera solutions are particularly challenging, since their description requires concepts from rather different fields of mathematics. Theory of synchronization has to be combined with ideas from pattern formation, deterministic chaos, and statistical physics. We will now introduce some basic ideas from these fields and then show how they can help to understand the chimera states.

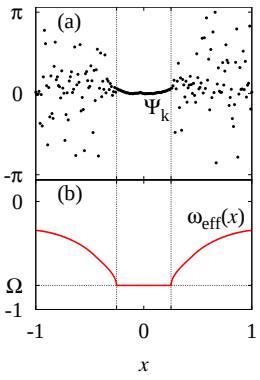


Fig. 2: *Chimera solution in system (4): phase snapshot (a), and the corresponding time-averaged phase velocities (b)*

Synchronization of coupled oscillators

Collective synchronization occurs in a huge variety of biological, chemical, physical, and social systems, therefore, it has attracted the interest of scientists for centuries. Chirping crickets, pedestrians on a bridge, or pulsing lasers can adjust their rhythms as a result of collective mutual interactions. The result might be helpful, like, e.g., the synchronization of oscillating semiconductor lasers in an optoelectronic communication system, or harmful, like in epileptic seizures where too many neurons in the brain get synchronized.

In a mathematical context, all such synchronization phenomena share many properties that can be described by systems of coupled oscillators. Since synchronization involves mainly the phases of the oscillators, one even can neglect the amplitudes and study systems of coupled phase oscillators. As a simple model of this type that can explain a lot of basic phenomena, the Japanese physicist Y. Kuramoto [2] has proposed in 1975 a system of the form

$$\frac{d\Psi_k}{dt} = \omega_k - \frac{K}{N}\sum_{j=1}^{N}\sin(\Psi_k(t) - \Psi_j(t)), \qquad k = 1, \ldots, N. \tag{1}$$

Without coupling (i.e., $K = 0$), each oscillator phase Ψ_k would run at its own frequency ω_k. But due to the coupling, there is an interaction force between any two oscillators that vanishes

only when their phases become equal, i.e., when they synchronize. On the other hand, for many coupled oscillators the sum of these forces could also almost vanish due to a compensation in the average. In this case, the system is in an asynchronous state of incoherent motion. To quantify the degree of synchrony in the system, Kuramoto introduced the macroscopic quantity

$$Z(t) = \frac{1}{N}\sum_{j=1}^{N} e^{i\Psi_j(t)}, \tag{2}$$

called the *complex mean field* that is able to indicate the transition from *incoherent* states with $|Z(t)| \approx 0$ to *coherent* (synchronized) states with $|Z(t)| \sim 1$ when the coupling K grows; see Figure 3. Analyzing the system (1) in the thermodynamic limit $N \to \infty$, Kuramoto pointed out that there exists a critical threshold $K_c = 2/[\pi g(0)]$ that is related to the probability distribution $g(\omega)$ of the natural frequencies ω_k. For coupling strength $K < K_c$, the oscillators are incoherent and act as if they were uncoupled: their phases Ψ_k remain uniformly distributed and, hence, the average $|Z(t)|$ is close to zero. When K exceeds K_c, there is an immediate transition to synchrony that first includes only oscillators with frequencies close to the average frequency (partial synchrony) and then gradually transforms into complete synchrony of all oscillators with a mean field $|Z(t)| = 1$.

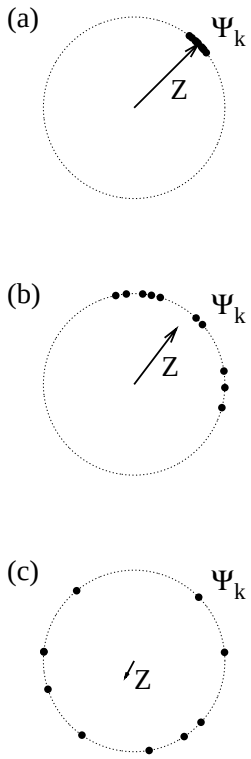


Fig. 3: *Geometric interpretation of the complex mean field for coherent (a), partially coherent (b) and incoherent (c) states*

Pattern formation in spatially extended systems

The emergence of patterns in a homogeneous environment is ubiquitous in nature. Ranging from the segmentation and morphogenesis in the development of simple organisms up to the stripes of a tiger, spontaneous pattern formation is a fascinating phenomenon that seems to be counterintuitive and inconceivable by a mathematical theory. However, in 1951 the British scientist A. Turing found a way to a mathematical treatment of such phenomena. He explained in his groundbreaking article "The chemical basis of morphogenesis" how in a system of interacting chemical species the interplay of diffusion and mutual chemical reactions can lead to the emergence of stable patterns from near-equal initial distributions. Up to now, this theoretical approach has been successfully applied to investigate many pattern-forming systems, in particular in chemical or biological systems. But a straightforward explanation of the synchrony patterns in chimera states can no longer be obtained in this way. The reasons for this are twofold:

— With the emergence of a Turing pattern, the homogeneous state becomes unstable. In contrast to that, the chimera states typically coexist with a homogeneous completely synchronized state.

— The concept of diffusion is based on continuously varying quantities in a continuous medium. But incoherent motion of coupled oscillators means that nearby units can show completely independent behavior.

Instead, as a further ingredient, we have to employ some theory about chaotic motion in deterministic systems.

Deterministic chaos

A system of differential equations like (1) is completely deterministic. Having specified an exact initial condition, there is a unique solution representing the time evolution over an arbitrary long time span. It was one of the fundamental discoveries of mathematics in the 20th century that the behavior of such systems can be still irregular and pretty unpredictable. The reason for that is the presence of so-called *dynamical chaos*. It manifests itself as a huge variety of possible complex motions in the system where arbitrarily small changes in the initial conditions lead already after a rather short time to wildly differing outcomes. As we will see below, this sensitive dependence on initial conditions is a fundamental property of the incoherent motion in a chimera state. But chaos is not a mathematical dead end. It is a point beyond which one needs to speak another language, related to irregular, unpredictable behavior of a dynamical system. In particular, chaos can be quantified by Lyapunov exponents, a measure of how quickly small initial differences diverge, i.e., a positive Lyapunov exponent is a signature of chaos and measures the degree of chaoticity.

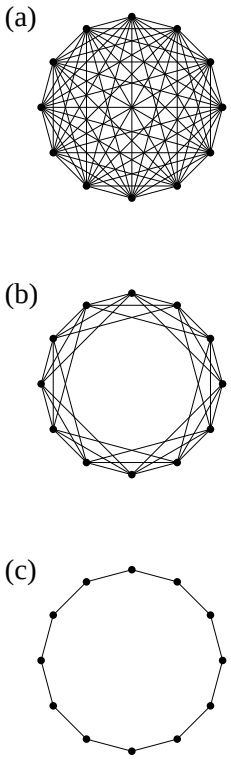


Fig. 4: *Different coupling topologies in a ring of oscillators: global (a), nonlocal (b), and local (c) coupling schemes*

Dynamical properties of chimera states

In order to find chimera states, we only have to introduce two small changes into Kuramoto's fundamental model (1): a nonlocal coupling structure and a phase lag in the sinusoidal coupling function. Instead of the global all-to-all coupling structure (see Figure 4(a)) of the original Kuramoto system, we arrange the oscillators as a ring where only a certain number of nearest neighbors interact (Figure 4(b)). But the coupling should also not be local with an interaction only between direct neighbors (Figure 4(c)). The phase lag is introduced by a parameter α in the coupling term $\sin(\Psi_k - \Psi_j + \alpha)$ and leads to a certain amount of repulsion between the oscillators. Indeed, for $\alpha > \pi/2$, the repulsion is large enough that the completely synchronized state loses its stability. In order to find chimera states, this parameter has to be carefully tuned to a value close but smaller than $\pi/2$. As a result, we obtain the system

$$\frac{d\Psi_k}{dt} = \omega - \frac{2}{N}\sum_{j=k-R}^{k+R} \sin(\Psi_k(t) - \Psi_j(t) + \alpha), \qquad k = 1, \ldots, N, \tag{3}$$

where R is the coupling range, and indices are considered modulo N (i.e. $N + 1 \equiv 1$). Note that all oscillators are here completely identical and have the same natural frequency ω. Solving this system numerically, we can observe chimera solutions as depicted in Figure 2(a). Along the horizontal axis, the $N = 200$ oscillators are equally distributed within the interval $x \in [-1, 1]$. The vertical axis displays their phases in the interval $[-\pi, \pi]$. The figure shows a single fixed time moment where the phases of incoherent oscillators are spread over the whole interval $[-\pi, \pi]$, whereas the coherent oscillators have similar phases and move synchronously. Consequently, all coherent oscillators have the same phase velocity. Due to their irregular motion, the incoherent oscillators do not have an equal constant phase velocity. But if we average their phase velocity, we obtain the continuous curve shown in Figure 2(b) that again displays nicely the two different regions. The chaotic nature of the chimera states turns out to be twofold. At first, the motion of each incoherent oscillator is chaotic. But in our recent research [4], we showed that also the region of incoherent motion itself shows a chaotic motion of its position.

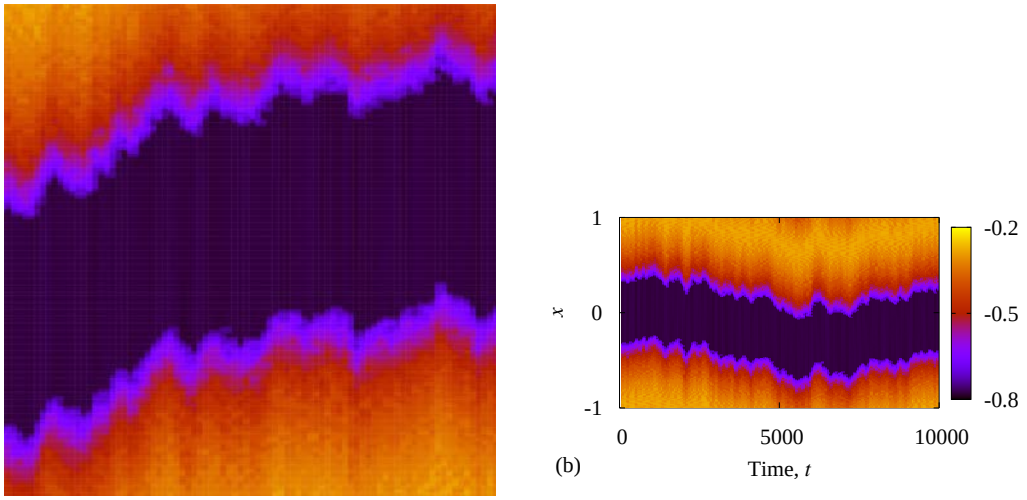


Fig. 5: *Sensitive dependence on initial conditions: two chimera trajectories with initial conditions that differ only by* 10^{-3}

Figure 5 shows two chimera trajectories by their color-coded time-averaged phase velocities. The coherent region (dark color) shows an irregular motion along the x-direction (here in vertical direction) depending sensitively on the initial conditions, which are chosen here to be nearly identical for both solutions. We have shown that for large N this lateral motion has the stochastic character of a Brownian motion. This reveals that chimera solutions are in fact spatio-temporal synchrony patterns with an irregular motion in space.

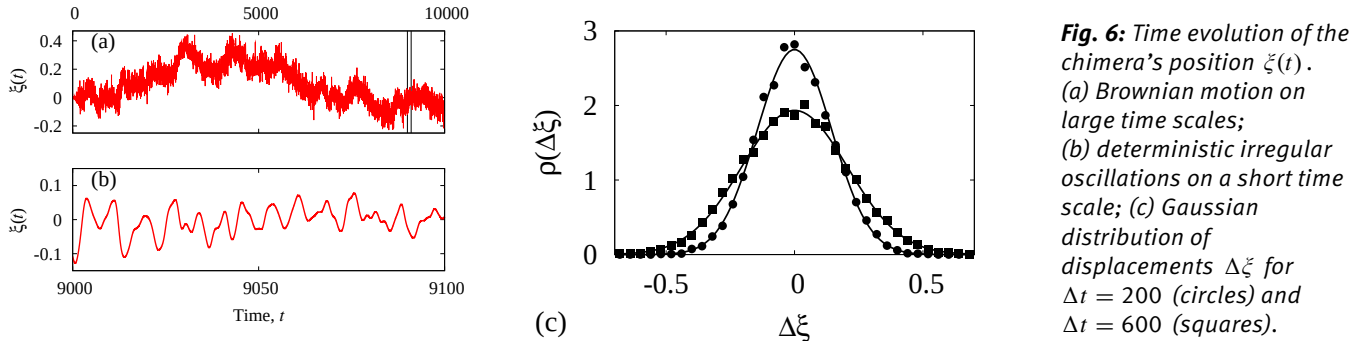


Fig. 6: *Time evolution of the chimera's position* $\xi(t)$. *(a) Brownian motion on large time scales; (b) deterministic irregular oscillations on a short time scale; (c) Gaussian distribution of displacements* $\Delta\xi$ *for* $\Delta t = 200$ *(circles) and* $\Delta t = 600$ *(squares).*

The chaoticity of the chimera states can also be revealed by the Lyapunov spectrum. Our calculations (see Figure 7) show a large number of positive Lyapunov exponents that indicate the existence of a chaotic attractor with a dimension that corresponds to the number of incoherent oscillators.

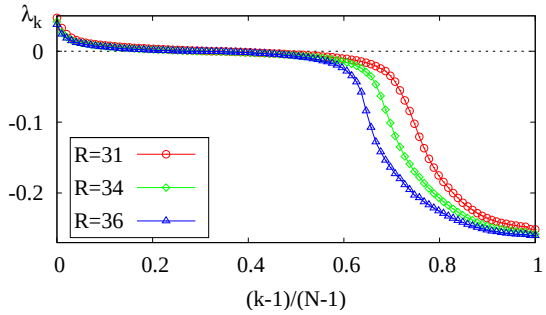


Fig. 7: *Lyapunov spectra λ_k computed for chimera trajectories of (3) with $N = 100$ and $\alpha = 1.44$. Different values of R lead to different sizes of the coherent region.*

For large numbers of oscillators, chimera solutions turn out to be statistically stationary states and they can be characterized with the help of averaged macroscopic quantities. To perform correctly the thermodynamic limit $N \to \infty$, we have to introduce a macroscopic coupling function $G(x)$, referring to the macroscopic positions $x_j = -1 + 2j/N$ of the oscillators. For the resulting system

$$\frac{d\Psi_k}{dt} = \omega - \frac{2}{N}\sum_{j=1}^{N} G(x_k - x_j)\sin(\Psi_k(t) - \Psi_j(t) + \alpha), \qquad k = 1, \ldots, N, \tag{4}$$

one can study the limit $N \to \infty$. For this, one needs to introduce a local complex mean field $z(x,t)$ similar to (2). This complex quantity represents the locally averaged behavior of oscillators in the vicinity of some point x. In particular, the identity $|z(x,t)| = 1$ means that the phase oscillators around point x are synchronized, while $|z(x,t)| = 0$ corresponds to a local absence of synchronization. It turns out that in the thermodynamic limit, the chimera states correspond to standing wave solutions $z(x,t) = \hat{z}(x)e^{i\Omega t}$ of the following integro-differential equation

$$\frac{\partial z}{\partial t} = i\omega z(x,t) + \frac{1}{2}Z(x,t) - \frac{z^2(x,t)}{2}Z^*(x,t), \quad \text{where } Z(x,t) = e^{-i\alpha}\int_{-1}^{1} G(x-y)z(y,t)\,dy. \tag{5}$$

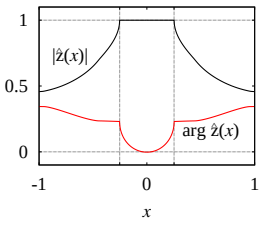


Fig. 8: *Complex amplitude of the standing wave solution to Eq. (5) corresponding to the chimera state in Figure 2*

Figure 8 displays a typical solution of Eq. (5) for the thermodynamic limit of a chimera state.

However, there are still no rigorous results in which sense the solutions of the thermodynamic limit equation can be understood as an approximation of a finite N-chimera.

References

[1] D.M. Abrams, S.H. Strogatz, *Chimera states for coupled oscillators*, Phys. Rev. Lett., **93** (2004), 174102.

[2] Y. Kuramoto, *Chemical Oscillations, Waves, and Turbulence*, Springer, Berlin, 1984.

[3] Y. Kuramoto, D. Battogtokh, *Coexistence of coherence and incoherence in nonlocally coupled phase oscillators*, Nonlin. Phenom. Complex Syst., **5** (2002), pp. 380–385.

[4] O.E. Omel'chenko, M. Wolfrum, Y.L. Maistrenko, *Chimera states as chaotic spatiotemporal patterns*, Phys. Rev. E, **81** (2010), 065201(R).

2.2 Random Numerical Methods for Simulating Soot Growth

Robert I. A. Patterson

Introduction

Soot forms as a result of the incomplete combustion of carbon-based fuels. Its chemical structure is partly like graphite, which is used for pencils, but it can also have large unstructured components, which are a little bit like tar. Soot is generally first seen as blue-black smoke emitted from a combustion device, for example, diesel engines in buses and aircraft engines.

Soot particles form when there is insufficient oxygen for the complete combustion of all the carbon in a fuel. As a result, some of the excess carbon is formed into large molecules (known as polycyclic aromatic hydrocarbons or PAHs), which then stick together to form soot particles. If the soot then passes through a hot, oxygen-rich region, it will start to burn and may be burned up completely. In this case, no soot will be seen from outside the combustion device. However, because soot particles are large collections of complex molecules, they burn rather slowly and can pass through hot oxidizing regions too quickly to be fully burned up.

The above description shows that soot forms very quickly and at conditions that are far from equilibrium. Physical models need to reflect the variety of soot particles that can form and their complex structure. However, traditional numerical techniques for differential equations are generally only capable of solving very simple models for soot particle formation and growth. Monte Carlo simulations using pseudo-random numbers provide a tool for scientists to calculate the predictions of realistic soot models so that they can be compared to experimental data.

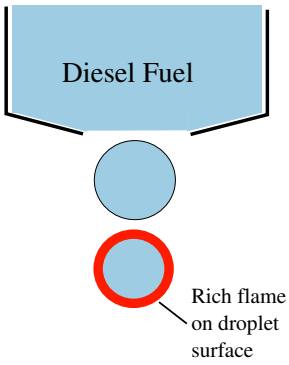


Fig. 1: *Soot forms in rich surface flames*

Modeling of soot particles

Diesel engines tend to produce soot, because fuel is sprayed into the cylinder in (very) small droplets. As the mixture in a cylinder is compressed, combustion starts at the interface between the fuel droplet and the surrounding oxygen-rich air, as illustrated in Figure 1. At this interface, a shortage of oxygen can develop and lead to soot formation. Petrol engines, which are generally less fuel efficient than diesel engines, avoid the particular problem of soot formation by premixing fuel vapor and air so that there are no droplet interfaces where soot can form.

Once soot particles have been formed (incepted), they can grow, shrink, and stick together (coagulate) to form larger particles. This leads to particles with interesting shapes and internal chemical structures. Mathematically, particles are described by elements of a "type space" $\mathcal{X}$ that can be defined to contain an appropriate level of physical detail for each problem. This level of detail will depend on the goals and the available computational resources. The potential complexity of a detailed geometric description can be seen in Figure 3.

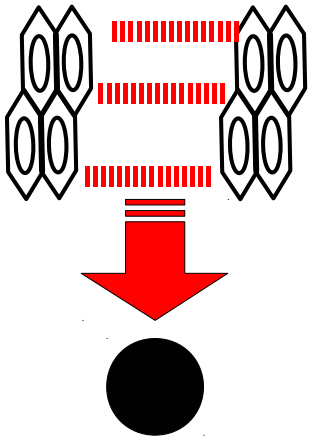


Fig. 2: *Particles form when two PAH molecules stick together due to attractive forces; the new particle is modeled as a sphere*

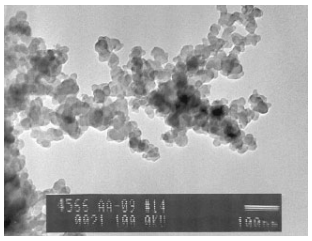


Fig. 3: *Transition Electron Micrograph of soot aggregate composed of primary particles (National Institute of Health, USA)*

A summary of the model for soot particles is now given:

1. Soot particles are incepted as spheres containing 32 carbon atoms at a rate I, which depends on the precalculated chemical species concentrations.
2. Each soot particle of type x coagulates with particles of type y at rate $K(x, y)$. The form of K used is the "transition regime kernel" as described in more detail in [1].
3. Pyrene molecules (16 carbon atoms, hydrogen is ignored) condense on the surface of soot particles of type x at rate $\beta_1(x)$, the new particle type is $g_1(x)$.
4. Acetylene molecules react with the surface of a soot particle of type x at rate $\beta_2(x)$, causing the particle to grow by 2 carbon atoms; the new particle type is $g_2(x)$.
5. Oxygen molecules react with the surface of a soot particle of type x at rate $\beta_3(x)$, causing the particle to lose 2 carbon atoms; the new particle type is $g_3(x)$.
6. OH radicals react with the surface of a soot particle of type x at rate $\beta_4(x)$, causing the particle to lose 1 carbon atom; the new particle type is $g_4(x)$.

This leads to the following equation for the concentration c of particles of type x at time t:

$$\frac{\mathrm{d}}{\mathrm{d}t}c(t,x) = \frac{1}{2}\sum_{\substack{y,z\in\mathcal{X}:\\ y+z=x}} K(y,z)\,c(t,y)\,c(t,z) - c(t,x)\sum_{y\in\mathcal{X}} K(x,y)c(t,y) + \sum_{l=1}^{4}\left(\left(\sum_{\substack{y\in\mathcal{X}:\\ g_l(y)=x}}\beta_l(y)\,c(t,y)\right) - \beta_l(x)\,c(t,x)\right) + I(x)\,. \quad (1)$$

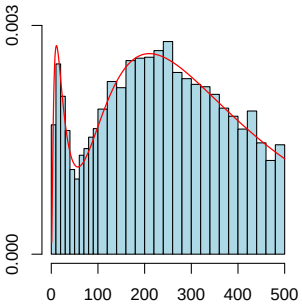


Fig. 4: *The true value of the particle distribution c is shown by the red line. The simulation procedure generates a list of particles, which are sampled (approximately) from this distribution. An estimate of c is then formed as a histogram.*

Stochastic numerical methods

Stochastic algorithms simulate the processes described above in a small sample volume, V. The sample volume has to be very small because every particle within it is individually tracked and its development is simulated according to the six points given above. In a stochastic algorithm, $c(t,x)$ is approximated by a list of particles $x_1(t), x_2(t), \ldots, x_{N(t)}(t) \in \mathcal{X}$ in the sense that, for smooth bounded functions $f\colon \mathcal{X} \to \mathbb{R}^+$,

$$\frac{1}{V}\sum_{i=1}^{N(t)} f(x_i(t)) \approx \sum_{x\in\mathcal{X}} f(x)c(t,x)\,, \quad (2)$$

provided that V is not too small. There is a tradeoff between choosing V small to make the list of particles short so that simulations run quickly and making V large enough so that the approximation equation (2) is good. For an alternative way of thinking about this approximation, see Figure 4.

For simple particle models, stochastic methods require greater amounts of computer power than other methods not based on particle lists. For example, it would not be practical to study droplets in a turbulent flow using stochastic particle methods, but using other methods, the problem can

be studied [2]. The advantage of stochastic methods is that they readily extend to problems when the structure of particles must be considered, which can be seen to be important for soot particles such as the one in Figure 3.

In principle, a stochastic algorithm has to simulate the time of every possible event for every particle and then perform only the first such event, before resimulating all the event times. The usefulness of stochastic algorithms depends on a number of mathematical and algorithmic techniques that greatly reduce the amount of recalculation.

Optimizing the simulation

Simulation of coagulation event times is particularly challenging, because every particle can coagulate with every other particle, giving $N(t)\,(N(t)-1)\,/2$ possible events each with its own rate. It is not practical to consider each event separately, even for $N(t)$ as small as 1,000, there are almost 500,000 pairs. However, a few basic ideas from probability theory allow the problem to be changed into one where one never has to consider more than $N(t)$ items at once.

The first idea is that instead of simulating the time to each possible coagulation event and then finding out which is the first, one can add up all the rates, use the sum to simulate the time at which something happens, and then choose between the possible pairs of particles that might have coagulated. This means that the overall coagulation events occur at rate

$$\sum_{i=1}^{N(t)} \sum_{j=i+1}^{N(t)} K(x_i, x_j). \tag{3}$$

The second idea is that one can generate coagulation rates at a higher rate and just throw away the excess events. Suppose that the rate is r; this means that the probability of a coagulation happening during a small time interval δt is approximately $r\delta t$. If the rate is increased to r/p for some p in the interval $(0, 1)$, then the probability of a coagulation in the same small interval is $r\delta t/p$. However, if these coagulations are ignored with probability $1-p$ so that only p of them go ahead, the probability of a coagulation really happening is reduced back to $r\delta t$. To exploit this possibility, choose a pair of functions k_1 and k_2 such that

$$K(x_i, x_j) \le k_1(x_i)k_2(x_j) + k_2(x_i)k_1(x_j). \tag{4}$$

For each pair i, j, choose a value of p

$$p_{ij} = \frac{K(x_i, x_j)}{k_1(x_i)k_2(x_j) + k_2(x_i)k_1(x_j)}. \tag{5}$$

Combining equations (3) and (4) shows that

$$\sum_{i=1}^{N(t)} \sum_{j=i+1}^{N(t)} K(x_i, x_j) \le \frac{1}{2} \sum_{i,j=1}^{N(t)} \left[k_1(x_i)k_2(x_j) + k_2(x_i)k_1(x_j)\right] = \lambda. \tag{6}$$

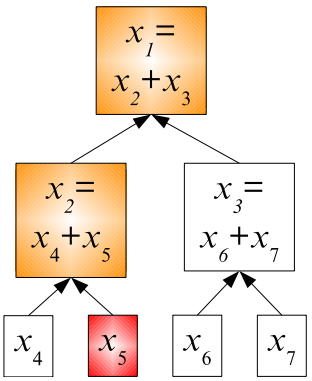


Fig. 5: *A binary tree is a very efficient way of keeping track of the sum of many numbers, which change one at a time. For example, when x_5 (highlighted in red) changes, only two additions have to be performed (the orange entries) to make x_1 correct again. For a tree with 1,000,000 entries, only 20 additions would be required when one entry changed.*

The algorithm to take one step is

1. Calculate $\lambda_1 = \sum_{i=1}^{N(t)} k_1(x_i)$ and $\lambda_2 = \sum_{i=1}^{N(t)} k_2(x_i)$. (So that $\lambda = \lambda_1 + \lambda_2$.)
2. Wait for a random time τ, which has an exponential distribution with mean $1/\lambda$.
3. Choose i according to the probabilities $k_1(x_i)/\lambda_1$ and j according to the probabilities $k_2(x_j)/\lambda_2$.
4. If $i = j$, go back to 1, and take another step.
5. With probability

$$1 - \frac{K(x_i, x_j)}{k_1(x_i)k_2(x_j) + k_2(x_i)k_1(x_j)}, \tag{7}$$

   go back to 1, and take another step.

6. The particles i and j coagulate. End of step.

Binary trees provide a very efficient way of calculating and updating these sums; they are briefly illustrated in Figure 5.

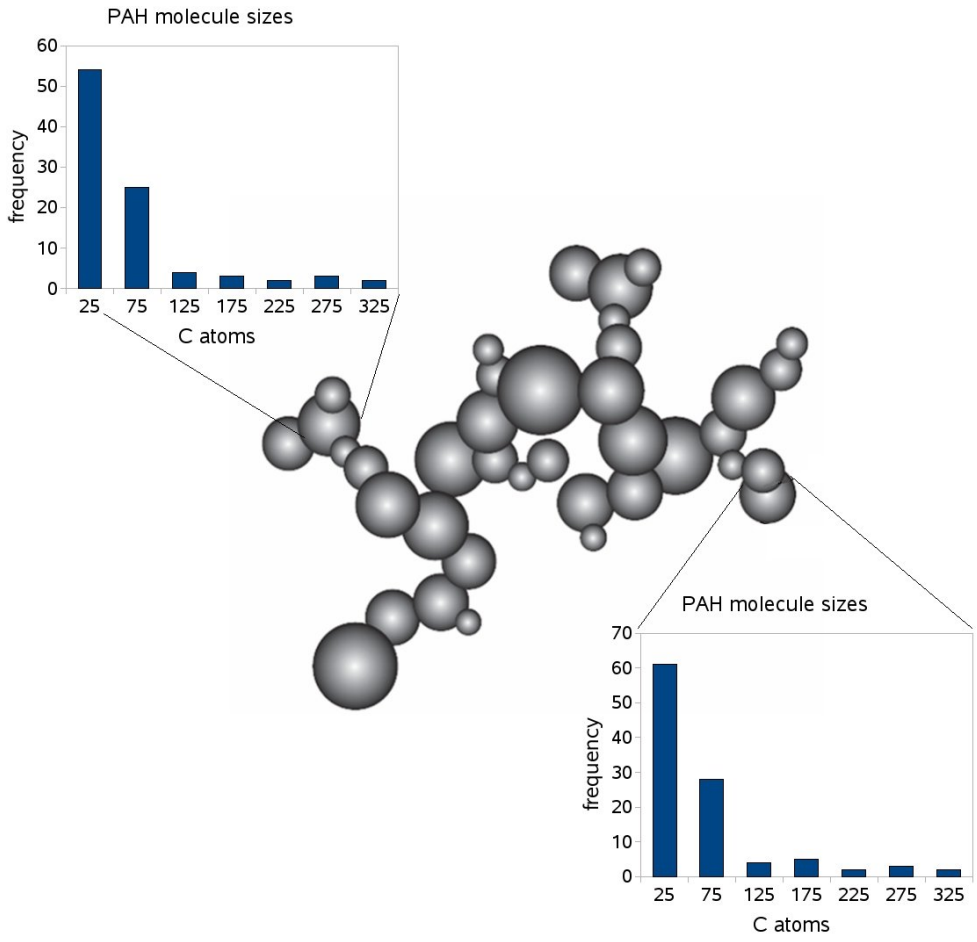


Fig. 6: *Soot particle modeled as collection of primary particles made up of PAH molecules whose sizes were part of the simulation; a list of which primary particles touch each other was also generated by the simulation*

Power of stochastic particles

Because stochastic particle methods store the particles in a volume V in a list rather than trying to discretize the space of all possible particles, it is easy to store extra details for each particle. Additional details have relatively little impact on the computational cost, because they do not change the number of particles or the number of events. As a consequence, stochastic particle methods can be used with very detailed models of soot particles in order to help understand the chemistry of soot formation in a way that is generally not possible with standard numerical methods for differential equations. For example, one can store the subunits (*primary particles*) that make up a soot particle and the connections between them as well as tracking the sizes of the PAH molecules that make up each primary particle [3]. With such a particle representation, a soot model can be expressed in terms of molecular reaction rates and simulated directly without having to simplify the model in order to make it compatible with another numerical method. One such simulated particle is shown in Figure 6.

In most situations, soot particles flow through a larger system. If the details of the systems are known in advance, this can be modeled by making the β_i and K change with time to reflect particle positions. However, because reactions between soot particles and the surrounding gas often have a significant effect on the gas, accurate results require the soot and the gas to be simulated together across the full spatial extent of the system. Simulation methods for the Boltzmann equation, where momentum takes the role played by mass in coagulation, are well developed [4]. Little is known about the simulation of coagulating particles in flows using stochastic particle methods. However, the basic idea of particles that move through a series of grid cells in which they coagulate can be used.

References

[1] R.I.A. Patterson, J. Singh, M. Balthasar, M. Kraft, W. Wagner, *Extending stochastic soot simulation to higher pressures*, Combust. Flame, **145** (2006), pp. 638–642.

[2] V. John, M. Roland, *On the impact of the scheme for solving the higher dimensional equation in coupled population balance systems*, J. Numer. Methods Engrg., **82** (2010), pp. 1450–1474.

[3] M. Sander, R.I.A. Patterson, A. Braumann, A. Raj, M. Kraft, *Developing the PAH-PP soot particle model using process informatics and uncertainty propagation*, Proc. Combust. Inst., **33** (2011), pp. 675–683.

[4] M.A. Gallis, J.R. Torczynski, D.J. Rader, G.A. Bird , *Convergence behavior of a new DSMC algorithm*, J. Comput. Phys., **228** (2009), pp. 4532–4548.

2.3 Quantum Graph Hamiltonians and Boundary Triplets

Hagen Neidhardt

Quantum graphs are important tools to model complex structures in different areas of physics, chemistry, and engineering. They naturally arise as simplified models of quantum mechanics when one considers the propagation of waves of various nature through a quasi-one-dimensional system, which looks like a neighborhood of a graph. In a more mathematical sense, a quantum graph is a network-shaped structure of vertices connected by edges with a differential or pseudo-differential operator acting on functions defined on the edges; see Figure 1. In quantum mechanics, these operators are called Hamiltonians. Thus, "quantum graph" is a shorthand for a Hamiltonian (operator) defined on a graph. Quantum graphs have become prominent models in mesoscopic physics used to obtain a theoretical understanding of nanotechnological devices.

They were first employed in the 1930s by Pauling to describe the spectrum of free electrons in organic molecules like naphthalene. The vertices are given by the atoms, while the bonds form edges that fix a frame in the shape of the molecule on which the free electrons are confined. Quantum graphs embedded in two or three dimensions appear in the study of photonic crystals. Waveguides are, in fact, fattened graphs where the edges are thin tubes with a width of some nanometers. Therefore, quantum graphs are used to model waveguides. Furthermore, quantum graphs are used for studying the appearance of quantum chaos. Periodic quantum graphs are of interest to understand the phenomena of the so-called *Anderson localization*. In the Research Group *Partial Differential Equations*, the interest in quantum graphs arises from the study of quantum transport of electrons through nanostructures, in particular through nanowires, which can be regarded as waveguides; cf. [1, 2, 3].

All these physical phenomena can be described by Hamiltonians (operators) living on the graph. Essential physical properties, like existence of bound states, discrete eigenvalues, energy spectrum, electronic band structure and gaps if the graph is periodic, conductivity, current density and charge density, resonances, etc., are encoded in the Hamiltonian, in particular, in its spectral properties. Thus, the spectral analysis of graph Hamiltonians is one of the main problems.

Quantum graphs and their Hamiltonians

A graph $\mathcal{G}$ consists of a finite or countably infinite set of vertices $\mathcal{V} = \{v_j\}$ and edges $\mathcal{E} = \{e_j\}$, which connect the vertices. A graph $\mathcal{G}$ is called a *metric graph* if each of its edges $e \in \mathcal{E}$ is assigned a positive length $l_e \in (0, \infty]$. Edges of infinite length are explicitly allowed. In our case, the edges are identified with intervals I_e of the real axis of length l_e; see Figure 1 for a typical example. In general, edges like loops, arcs, etc., are not excluded; however, we omit them for simplicity. Identifying e with intervals I_e, one introduces the Hilbert space $L^2(\mathcal{G})$ that consists of square integrable functions on each edge e with values in the set of complex numbers $\mathbb{C}$, that is, $f = \{f_e\}_{e\in\mathcal{E}}$, $f_e : I_e \longrightarrow \mathbb{C}$ such that

$$\|f\|^2_{L^2(\mathcal{G})} = \sum_{e\in\mathcal{E}} \|f_e\|^2_{L^2(e)} < +\infty.$$

In other words, $L^2(\mathcal{G})$ is the orthogonal direct sum of the spaces $L^2(e) = L^2(I_e)$, $e \in \mathcal{E}$.

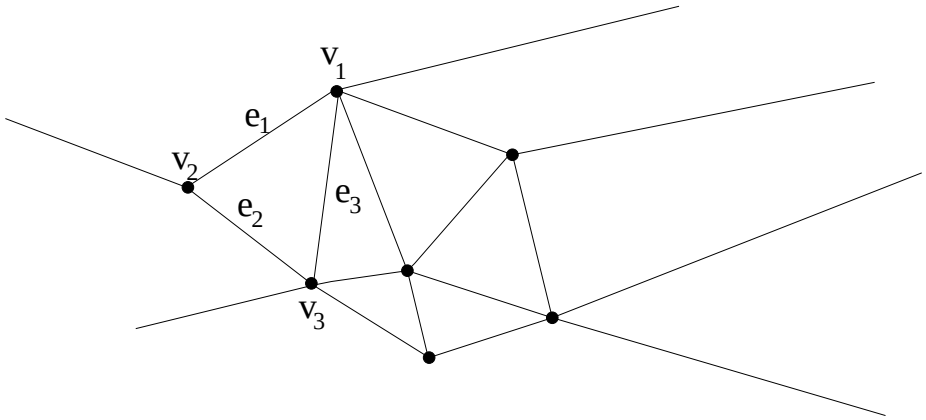


Fig. 1: *Example of quantum graph*

In order to make a matric graph a quantum graph, one has to give for each edge $e \in \mathcal{E}$ a differential operator. Frequently used edge operators H^e are the following ones:

$$H^e_{\text{Laplace}}: \quad f_e(x) \longrightarrow -\frac{d^2 f_e}{dx^2}, \quad e \in \mathcal{E}, \tag{1}$$

$$H^e_{\text{Schr}}: \quad f_e(x) \longrightarrow -\frac{d^2 f_e}{dx^2} + V_e(x) f(x), \quad e \in \mathcal{E}, \tag{2}$$

$$H^e_{\text{magnetic}}: \quad f_e(x) \longrightarrow \left(i\frac{d}{dx} - A_e(x)\right)^2 f_e(x) + V_e(x) f(x), \quad e \in \mathcal{E}, \tag{3}$$

called *Laplace, Schrödinger-type*, and *magnetic Schrödinger-type operator*, where the real function $V(x)$ is called the *potential* that is usually assumed to be decaying at infinity on edges with infinite length, and A_e is the electromagnetic potential. In general, it is assumed that their domains $\mathrm{dom}(H^e)$ are the set of smooth functions that are identical zero in a neighborhood of vertices called the *minimal domain*. The maximal domain is simply the set of smooth functions.
All these Hamiltonians are semibounded from below. However, more general Hamiltonians occur that are not semibounded. This is the case for graphene that was discovered by Boehm in 1962. In 2010, the Nobel Prize in Physics was awarded to Geim and Novoselov for "groundbreaking experiments regarding the two-dimensional material graphene"[1]. In contrast to the examples above, graphene requires to use the Dirac operator

$$H^e_{\text{graph}}: \quad \vec{f}_e(x) \longrightarrow \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \frac{d\vec{f}_e}{dx}(x) + \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix} \vec{f}_e(x), \quad a \in \mathbb{R}, \quad e \in \mathcal{E}, \tag{4}$$

that is not semibounded from below! The graph structure of graphene can be seen in Figure 2. Of course, more complicated scalar or even matrix differential operators as well as pseudo-differential operators were also investigated.

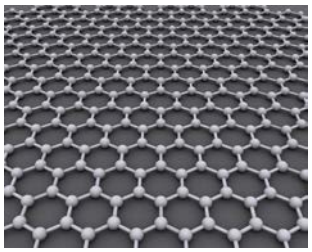


Fig. 2: *Graph structure of graphene*

The fundamental requirement for Hamiltonians in quantum mechanics is their self-adjointness that, in particular, implies that the spectrum is real. Roughly speaking, a self-adjoint operator

[1] Nobel Foundation announcement

is a symmetric operator that does not admit any symmetric extension; it is in some sense maximal. The edge operators H^e are symmetric, but not self-adjoint, which yields that the direct sum $H := \bigoplus_{e\in\mathcal{E}} H^e$ is as well a symmetric operator in the Hilbert space $L^2(\mathcal{G})$. The requirement of self-adjointness leads to the problem to consider self-adjoint extensions of H what for quantum graphs is equivalent to choose appropriate vertex conditions. A vertex condition links the boundary values of functions $f_e(v)$ of the maximal domains of the edge operators H^e and of their derivatives $\frac{df_e}{dx_e}(v)$ at the vertices $v \in \mathcal{V}$ in such a way that the resulting operator on the graph is self-adjoint. A self-adjoint extension $\widetilde{H}$ of H is called a *graph Hamiltonian*. All physical properties of a quantum graph are hidden in it. The vertex condition reflects how the edges interact. Of course, the graph Hamiltonian is not uniquely determined, since the symmetric operator H admits a lot of self-adjoint extensions that correspond to different vertex conditions. In principle, a vertex condition can mix the values at different vertices. However, in applications vertex conditions are local, that is, they mix only values of the same vertex. A typical vertex condition is the so- called *Kirchhoff condition*: the function $f = \{f_e\}_{e\in\mathcal{E}}$ is continuous on $\mathcal{G}$, and at each vertex $v \in \mathcal{V}$ the condition

$$\sum_{e\in\mathcal{E}_v} \frac{df_e}{dx_e}(v) = 0$$

is satisfied, where the sum is taken over all edges $\mathcal{E}_v$ incident to the vertex $v \in \mathcal{V}$. The derivatives are regarded as directed away from the vertex v. The name of this vertex condition is derived from the famous Kirchhoff junction rule of electric circuits. The vertex conditions are of great importance, since the graph Hamiltonian essentially depends on them, in particular, on their spectral properties and, therefore, on the physics of the quantum graph. With respect to nanostructures, we focus on the absolutely continuous spectral part of graph Hamiltonians that is related to the electron transport through the nanostructure. So the problem arises how this part of the graph Hamiltonian depends on the vertex conditions.

Boundary triplet approach to extension theory

From the viewpoint of operator theory, the situation of the quantum graph can be modeled as follows: we have a family of Hilbert spaces $\{\mathfrak{H}_e\}_{e\in\mathcal{E}}$, and in each of the Hilbert spaces $\mathfrak{H}_e$ there is given a symmetric operator H^e that is not self-adjoint. Now, the direct sum $H = \bigoplus_{e\in\mathcal{E}} H^e$ defines a symmetric operator in $\mathfrak{H}$.

To describe the self-adjoint extensions of H we used the so-called *boundary triplet approach*. The advantage of this approach is a very convenient description of all possible self-adjoint extensions, which is an excellent prerequisite for the investigation of the spectral properties of graph Hamiltonians. In more detail, for any arbitrary symmetric operator H, the boundary triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ consists of a boundary value space $\mathcal{H}$, which is a Hilbert space, and two linear boundary maps $\Gamma_i : \mathrm{dom}(H^*) \longrightarrow \mathcal{H}$, which assign boundary values to elements of the domain $\mathrm{dom}(H^*)$ of the adjoint operator H^*. The operator H^* and the maps Γ_i have to satisfy Green's identity

$$(H^* f, g) - (f, H^* g) = (\Gamma_1 f, \Gamma_0 g) - (\Gamma_0 f, \Gamma_1 g), \quad f, g \in \mathrm{dom}(H^*),$$

and the boundary value space $\mathcal{H}$ has to exhaust all possible boundary values.

One chooses now a boundary triplet $\Pi^e = \{\mathcal{H}^e, \Gamma_0^e, \Gamma\}$ for each symmetric operator H^e and defines the boundary triplet of the whole operator $H = \bigoplus_{e\mathcal{E}} H^e$ as the direct sum of the individual boundary triplets, that is, $\Pi = \bigoplus_{e\in\mathcal{E}} \Pi^e$. Having defined a boundary triplet for a symmetric operator H, it turns out that for any self-adjoint extension $\widetilde{H}$ of H there is a self-adjoint boundary operator B in the boundary value space $\mathcal{H}$ such that the domain $\mathrm{dom}(\widetilde{H})$ of the extension $\widetilde{H}$ is given by $\mathrm{dom}(\widetilde{H}) = \{f \in \mathrm{dom}(H^*) : \Gamma_1 f = B\Gamma_0 f\}$, where $\mathrm{dom}(H^*)$ is the domain of the adjoint operator. In fact, this correspondence is bijective. Among all self-adjoint extensions of a symmetric operator H, there is a special one H_∞ that corresponds to $B = \infty$ and has the domain $\mathrm{dom}(H_\infty) = \{f \in \mathrm{dom}(H^*) : \Gamma_0 f = 0\}$. In the present case, this leads to $H_\infty = \bigoplus_{e\in\mathcal{E}} H^e_\infty$.

There are symmetric operators that are very different from maximal symmetric or self-adjoint operators and other ones that are very close to them. Mathematically, this important property is expressed by saying that the deficiency indices are infinite or finite, respectively. Notice that even if the individual symmetric operators H^e have finite deficiency indices, it can happen that the direct sum $H = \bigoplus_{e\in\mathcal{E}} H^e$ has infinite deficiency indices!

Theorem 1 (Malamud and Neidhardt [4]) *Let $\{H^e\}_{e\in\mathcal{E}}$ and $\{H^e_\infty\}_{e\in\mathcal{E}}$ as well as H and H_∞ be given as above. If the symmetric operators H^e have only finite deficiency indices, then the absolutely continuous part of H_∞ is embedded into the absolutely continuous part of any self-adjoint extension $\widetilde{H}$ of H.*

Roughly speaking, the absolutely continuous part of H_∞ is a part of any self-adjoint extension of H. Hence, the absolutely continuous spectrum $\sigma_{ac}(H_\infty)$ of H_∞ is contained in the absolutely continuous spectrum $\sigma_{ac}(\widetilde{H})$ of any self-adjoint extension $\widetilde{H}$, i.e., $\sigma_{ac}(H_\infty) \subseteq \sigma_{ac}(\widetilde{H})$.

With respect to quantum graphs, the abstract results of operator theory apply as follows: we set $\mathfrak{H}_e = L^2(e)$, whilst the operators H^e are examples from above. The whole Hilbert space $\mathfrak{H}$ is the direct sum of the single Hilbert spaces, i.e., $\mathfrak{H} = \bigoplus_{e\in\mathcal{E}} \mathfrak{H}_e$ that coincides with $L^2(\mathcal{G})$ for quantum graphs. For each edge operator H^e, one defines a boundary triplet $\Pi^e = \{\mathcal{H}^e, \Gamma_0^e, \Gamma_e^1\}$. The boundary value space $\mathcal{H}^e$ actually consists of all boundary values of elements of the maximal domain and their derivatives at vertices belonging to the edge e, that is, of $\{f_e(v)\}$ and $\left\{\frac{df_e}{dx_e}(v)\right\}$. The maps Γ_0^e evaluate the functions f_e at the vertices belonging to e, and the map Γ_1^e evaluates the derivatives $\frac{df_e}{dx_e}$ at the vertices. Green's identity for each edge follows from integration by parts. The boundary value space $\mathcal{H} = \bigoplus_{e\in\mathcal{E}} \mathcal{H}^e$ of the direct sum $H = \bigoplus_e H^e$ is now the set of all boundary values $\left\{f_e(v), \frac{df_e}{dx_e}(v)\right\}_{e\in\mathcal{E}, v\in\mathcal{V}}$. Self-adjoint extensions of H are given by self-adjoint operators B acting on the set of boundary values. That means, for quantum graphs the operator B links the boundary values $\{f_e(v)\}_{e\in\mathcal{E},v\in\mathcal{V}}$ and $\left\{\frac{df_e}{dx_e}(v)\right\}_{e\in\mathcal{E},v\in\mathcal{V}}$ in an appropriate way. The problem of quantum graphs can be reformulated as follows: determine the spectral properties of the graph Hamiltonians for varying boundary operators B.

The special extensions H^e_∞ correspond for graphs to the so-called *Dirichlet extensions* $H^{e,D}$, $e \in \mathcal{E}$, the domain of which is given by all those elements of the maximal domain of H^e satisfying the Dirichlet boundary condition at the end of edges. Obviously, we have $H_\infty = H^D := \bigoplus_{e\in\mathcal{E}} H^{e,D}$. The Hamiltonian H^D is called the *Dirichlet Hamiltonian* of the graph. Physically, it corresponds to a totally decoupled graph that does not allow any electron transport through it.

A further important feature of quantum graphs is that the edge operators H^e have finite deficiency

indices. This follows from the observation that all example edge operators from above are, in fact, ordinary differential operators. With respect to quantum graphs, Theorem 1 tells us now that the absolutely continuous part of the Dirichlet Hamiltonian is a part of any graph Hamiltonian.

A natural problem in operator theory as well as in quantum graphs is to find as large a class of self-adjoint extensions as possible, for which the absolutely continuous parts coincide with the one of H_∞ up to unitary equivalence. It is possible to find such a class if one takes into account the notion of Weyl function. Similar to the theory of Sturm–Liouville operators on the real half-axis, for which an important tool is the so-called (scalar) *Titchmarsh–Weyl function*, one associates with each boundary triplet a so-called abstract *Weyl function* $M(\cdot)$, which is a holomorphic operator-valued function defined on the upper half plane $\mathbb{C}_+$ such that its imaginary part is nonnegative in the operator sense (Nevanlinna function). In general, Weyl functions do not admit boundary values at the real axis. However, if they do, then this has strong implications:

Theorem 2 (Malamud and Neidhardt [5]) *Assume that there is a boundary triplet for H such that the corresponding Weyl function admits weak boundary values for almost every point of the real axis. If B is a self-adjoint boundary operator with compact resolvent, then the absolutely continuous parts of H_B and H_∞ are unitarily equivalent.*

For quantum graphs, Theorem 2 has the following consequences:

Corollary 3 *Let the spectrum of the Dirichlet Hamiltonian H^D be discrete outside of its absolutely continuous spectrum $\sigma_{ac}(H^D)$. If the resolvent of the graph Hamiltonian $\widetilde{H}$ differs from that one of H^D by a compact operator, then the absolutely continuous parts of $\widetilde{H}$ and H^D are unitarily equivalent.*

Roughly speaking, vertex conditions cannot change the absolutely continuous parts of graph Hamiltonians as far as their resolvents differ from the resolvent of H^D by a compact operator.

References

[1] P. Exner, *Leaky quantum graphs: A review.*, in: Analysis on Graphs and its Applications, Proc. Sympos. Pure Math., **77**, Amer. Math. Soc., Providence, RI, 2008, pp. 523–564.

[2] P. Kuchment, *Quantum graphs. I. Some basic structures*, Waves Random Media, **14(1)** (2004), pp. S107–S128.

[3] P. Kuchment, *Quantum graphs: An introduction and a brief survey*, in: Analysis on Graphs and its Applications, Proc. Sympos. Pure Math., **77**, Amer. Math. Soc.,Providence, RI, 2008, pp. 291–312.

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

[5] M. M. Malamud, H. Neidhardt, *On the unitary equivalence of absolutely continuous parts of self-adjoint extensions*, J. Funct. Anal., **260** (2011), pp. 613–638 (first part of [4]).

2.4 Coupled Flow Processes in Energy and Environmental Research

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The efficient and accurate simulation of coupled flow processes is an important and in many cases not yet satisfactorily solved problem in fields like energy, climate, geological and environmental research. The Research Network "Coupled Flow Processes in Energy and Environmental Research" was established in the framework of a competitive procedure of the Leibniz Association. The network, coordinated by the Weierstrass Institute, brought together research groups from WIAS, the Freie Universität Berlin, the Potsdam Institute for Climate Impact Research (PIK), and the University of Erlangen during the funding period 2008–2010. Its main focus was on coupled flow processes in electrochemical systems like fuel cells and on the coupling between flow processes in the atmosphere and in the soil. New results were obtained both in the direction of method development and verification, as well as their application. Strong emphasis was placed on comparison with measured data.

A culminating moment of the project was the International Workshop "Coupled Models in Energy, Hydrology and Climate Research", which took place at WIAS on October 8–9, 2009. This workshop was jointly organized with the network "Adaptive Hydrological Modeling with Applications in Water Resource Management (AdaptHydroMod)" funded by the German Ministry of Education and Research.

We give a short overview of the main results of the project.

Mass conservative coupling in electrochemical processes (Weierstrass Institute)

A large part of the work in this field was dedicated to the further development and investigation of discretization schemes for the Navier–Stokes equation on unstructured meshes, which guarantee mass conservation and maximum principles for the discretization of the transport of a dissolved species that moves with the flow. These and other properties can be preserved under discretization of the transport equation by the Voronoi box based finite volume scheme on boundary-conforming Delaunay meshes if the projected velocity field is discretely divergence free in the sense that on every control volume, a discrete flow balance is fulfilled.

This property can be guaranteed in a natural way by choosing a pointwise divergence-free finite element for the Navier–Stokes equations and by calculating the discrete flow by exact integration over the control volume boundaries.

Based on this approach, a coupling scheme for fluid flow and species transport using the Scott–Vogelius mixed finite element for the Navier–Stokes equations was investigated, and its convergence was proven [1]. Further, a deeper understanding of the connections of the Scott–Vogelius element with grad-div stabilization approaches for the Taylor–Hood element was obtained [7]. A

number of numerical investigations resulted in examples where mass conservation is important for the flow itself [5].

While exhibiting a number of desired properties, calculations based on the Scott–Vogelius element are expensive. Therefore, another aim of the project was to develop generalizations of the staggered grid approach of the classical Marker-and-Cell (MAC) scheme to unstructured grids with the main property that the discrete mass balance equation coincides with the above-mentioned divergence condition for transport. In this direction, concepts and first steps towards implementation and convergence theory were obtained [3]. In this process, the convergence of a finite volume discretization of the biharmonic problem was established [6].

Fig. 1: *H_2 concentration in the cell is bounded by its value at the inlet when using the Scott–Vogelius element for the fluid flow. Right: H_2 concentration in the cell exceeds its value at the inlet when using the Taylor–Hood element.*

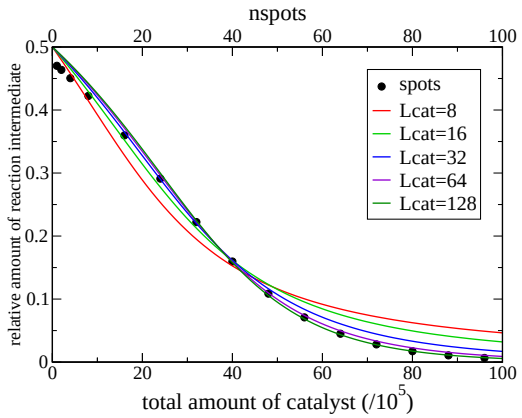


Fig. 2: *Fraction of intermediate in the products $B_{out}/(B_{out} + C_{out})$ depending on the total amount of catalyst N_{cat}. Left: results for fixed velocity and varying amounts of catalyst.*

Various variants of coupled systems in the field of electrochemistry were investigated. In particular, the previously described coupled finite element/finite volume scheme was successfully used to interpret a limiting current experiment in a cylindrical flow cell [4]. Figure 1 demonstrates the consequences of the use of different discretization schemes for the stationary Navier–Stokes equations. A correct calculation of the limiting current allows us to go further and to investigate the coupling of species flow and multistep catalytic surface reactions [2]. Since intermediate products of such

reactions may desorb from and re-adsorb to the catalytic surface, a certain amount of them can be found in the product stream. Experimental evidence shows a strong inverse correlation of the fraction of intermediates in the product stream with the amount of available catalyst sites. It is yet to be established if this effect is caused by micro- or macro-scale processes. We developed a macroscopic conceptual model of a three-stage reaction. Using this model, we achieved good qualitative coincidence with the experimental evidence; see Figure 2.

Polynomial chaos expansions in the stochastic Richards equation (Freie Universität Berlin)

While much effort has been invested into controlling and reducing the error arising from the discretization of partial differential equations and the numerical solution of the resulting discretized equations, the consequences of uncertainties in input data and model parameters have received less attention for a long time. The polynomial chaos approach combines the Galerkin approach inherent to the finite element method with a Galerkin approach for polynomial ansatz functions on a stochastic space derived from the Karhunen–Loeve expansion, a standard tool in the analysis of stochastic processes, to an efficient computational tool.

It allows one to establish expectations, variances, and other probabilistic characterizations of the solution depending on the uncertainties of the data. In particular, for this purpose, the polynomial chaos (PC) method is computationally more efficient than straightforward variants of the Monte Carlo method. It has been applied successfully to a broad range of applications [8] and has been mainly analyzed for linear elliptic problems resulting in stochastic variational equations.

The doubly nonlinear elliptic-parabolic Richards equation describes saturated-unsaturated flow in porous media. It is an established model for describing groundwater flow in soils. Due to the very nature of natural porous media like soils, a high degree of parameter uncertainty is inherent to this and any other modeling approaches.

Suitable transformations and an explicit-implicit time discretization scheme permit to rewrite Richards equation as a variational inequality of second kind, allowing its reformulation as a minimization problem [11].

This approach was sucessfully combined with the polynomial chaos method. For the numerical solution, a Galerkin ansatz was chosen and equivalence with a special case of stochastic collocation approaches [9] was shown. Based on this result, decoupling in a stochastic direction allows one to solve the spatial problems in a fast and reliable way by monotone multigrid methods.

The resulting model allows to characterize uncertainties in the soil saturation in terms of the uncertainties of permeability data.

The application of polynomial chaos to variational inequalities is rather new, and the development of the convergence theory was started [10]. Numerical experiments suggest similar convergence estimates as for the linear stochastic diffusion problem [9].

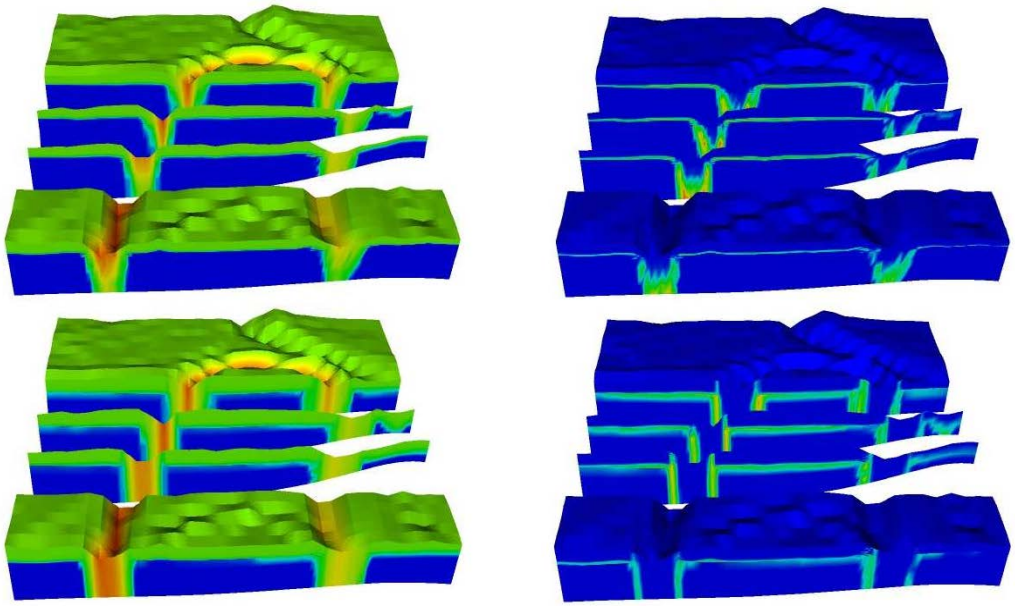


Fig. 3: *Infiltration of water from a river into originally dry soil for t=2000 (top), t=15000 (bottom). The left row shows the expectation, the right row the variance obtained using a PC basis of size 32. A lognormally distributed permeability with exponential covariance has been assumed.*

Sensitivity of a coupled boundary layer/atmosphere model to shear stress parameterization (Freie Universität Berlin)

The subproject was motivated by the need for new boundary conditions for the atmosphere-land surface interaction.

The interaction between the land surface and the free atmosphere takes place in the planetary (Ekman) boundary layer; a layer where the momentum equations are simply represented by a three-way balance between the forces due to Coriolis, pressure gradient, and friction [12]. However, there is a lack of agreement on the best way to represent friction in the layer, and several approaches have been suggested in the literature [12]. Also the characteristic features of the exchanges of momentum, heat, and matter transport, such as nonlinear interactions, spatial heterogeneities, and temporal fluctuations, need to be incorporated in the representations.

We solved the Ekman layer equations with various parameterization schemes. Initial results show that the surface friction velocity and the wind direction increase with increase in surface roughness. We have observed that changes in the geostrophic wind can lead to significant changes in the flow pattern and that the surface stress vector depends on atmospheric stability in the Ekman layer. These sensitivities of roughness length and geostrophic wind on the shear stress could have a profound effect on the Ekman pumping, a traditional way of representing the effects of surface friction on large-scale weather development. An investigation of the influence of the geostrophic wind and characteristics of the underlying surface in a three-level quasi-geostrophic (QG) model [13] reveals how sensitive the flow patterns are to the choice of the shear stress parameterization; see, for example, Figure 4. Finally, attempts were made to understand how the polynomial chaos approach methodology can be used to quantify the uncertainties in the shear stress due to the uncertainty in the surface roughness. Initial results were obtained that demonstrate the use of the

non-intrusive polynomial chaos approach [8] to propagate uncertainty in the roughness length in the Ekman layer model.

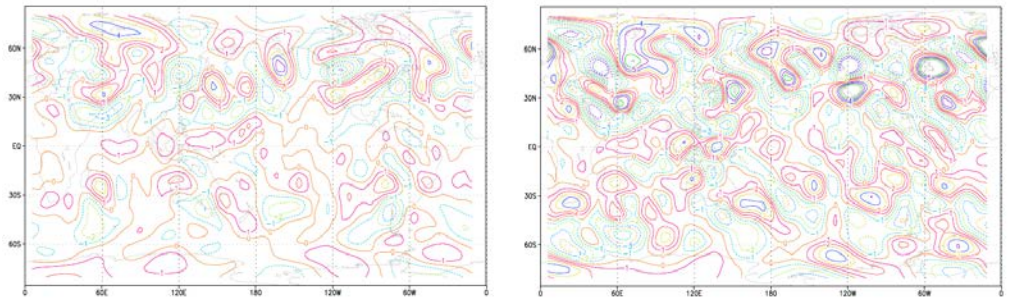


Fig. 4: *Influence of shear stress parameterization on vorticity contours in a quasi-geostrophic model. Shear stress* $\tau_x = K_m \partial_z u$, $\tau_x = K_m \partial_z v$. *Left:* $K_m = const$, *right:* $K_m = \updownarrow^2 |\vec{u}_z|$ *(von Karman mixing-length closure).*

River routing in a regional climate model (Potsdam Institute for Climate Impact Research)

In order to model and investigate floods and droughts in the context of climate simulations, an implementation of river routing is essential. River routing is a method to model the movement of a fluid wave through rivers and reservoirs that takes into account flow resistance and storage capacities. A mathematical model for this process is commonly derived from reasonable simplifications of the momentum transport for fluid flow.

In the framework of the project, at PIK Potsdam, river routing was implemented into the dynamical regional climate model “COSMO in CLimate Mode” (CCLM) of the German climate research community. It represents a non-hydrostatic model for weather and climate research. It can be used to simulate the climate at the mesoscale for up to decades, while handling resolutions down to a few kilometers [14].

To provide lower boundary conditions over land, it includes the land-surface parameterization scheme TERRA_ML [15]. TERRA-ML still has several shortcomings, such as a missing routing scheme, missing wetlands, or a rather crude representation of the vegetation dynamics. Implementation of the routing scheme started with the use of the soil and water integrated model SWIM [16], an ecohydrological model widely employed at PIK. SWIM was fine-tuned for the Elbe catchment and extensively evaluated for various aspects of the hydrological cycle.

A performance evaluation of TERRA-ML on pre-existing data yielded that, while precipitation and evaporation were decently reproduced, the reproduction of runoff was poor. This result had been expected since TERRA-ML lacked retention mechanisms.

SWIM uses the Muskingum routing scheme for the calculation of the flow through river reaches. Routing the surface and the subsurface runoff via the Muskingum scheme yielded suboptimal results on the data of the Elbe catchment.

Therefore, we implemented a ground water table into TERRA_ML. Now, the subsurface runoff trickles into the ground water table, and from there it is routed according to the Muskingum scheme.

This approach improved the routing performance considerably. Both the ground water table and the Muskingum routing introduce new parameters, which have to be tuned for the catchment under consideration.

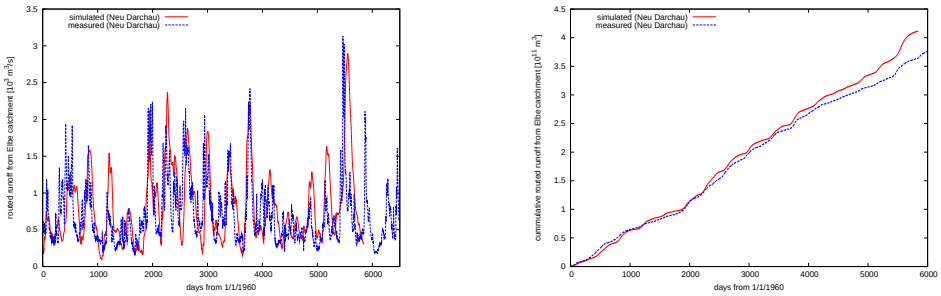


Fig. 5: *Measured (blue) and simulated (red), daily (left) and accumulated (right) runoff from the Elbe catchment at Neu-Darchau*

The results of the combination of a ground water table and the Muskingum routing are shown in Figure 5. In general, we are able to reproduce the main patterns and yearly peaks. The spikes, however, overshoot and are sometimes somewhat delayed. Simulated and measured accumulated runoffs match rather well for about the first ten years. After that, the observations and the simulation begin to deviate.

Even the improved routing still has considerable shortcomings, which might be atttibuted to missing models for snow and wetlands, thus calling for further investigations.

Multiphase flow with heat and mass transfer across the phase boundary (Erlangen University)

A particular case of coupling between fluid and gas flows occurs in the modeling of the behavior of cryogenic rocket propellants. In the presence of gravity, the influence of capillary effects on the behavior of the free surface between gas and fluid is usually small. However, during the rocket's long ballistic flight phases in space, gravity is absent, and capillary forces are the dominating factor influencing the dynamic behavior of the liquid. Since the surface tension is temperature dependent, temperature differences between the fluid and the container wall are the driving force for liquid flow (Marangoni effect). Based on a finite element model featuring a sharp interface between liquid and gaseous phase and vapor transport in inert gas, this effect and its interaction with evaporation were investigated numerically.

Experimental data is available from the French-German COMPERE project [22] between companies from space industry and academic institutions. In particular, data provided by the SOURCE experiment (SOunding Rocket COMPERE Experiment, [20]) conducted aboard MASER 11, a sounding rocket launched in Kiruna on May 15, 2008, served as a benchmark for the evaluation of commercial and academic computational fluid dynamics (CFD) codes. In this benchmark, a simplified experimental setup was designed in order to identify and to understand the underlying basic physical mechanisms [19] of fluid behavior in a two-species system under non-isothermal conditions.

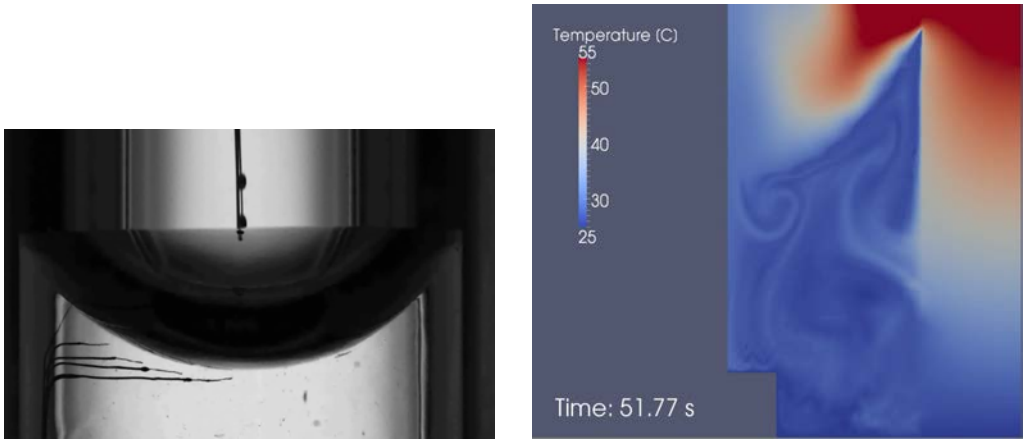


Fig. 6: *Unsteady Marangoni convection on hot wall under microgravity conditions. Left: SOURCE experiment. Right: Temperature distribution in the SOURCE experiment, simulated with NAVIER.*

For the numerical simulation of the SOURCE experiment, the academic code NAVIER [21] was extended by the ability to simulate two-phase flow (liquid, gas) and a model for evaporation and condensation. In the SOURCE benchmark, numerical predictions show good agreement with experimental findings and results obtained from commercial CFD solvers.

Under the influence of evaporation, the stability of the phase boundary is an important issue. A linear stability analysis was performed that showed that evaporation and the resulting loss of mass in the liquid phase has a destabilizing effect on the phase boundary [17]. This observation was confirmed and quantified by numerical simulations with NAVIER.

The current object of research is (in contrast to the two-species system SOURCE) the simulation of a single-species system (liquid argon and its vapor, [18]), where the driving force behind the dynamic behavior of the liquid is still unknown.

References

[1] J. Fuhrmann, A. Linke, H. Langmach, *A numerical method for mass conservative coupling between fluid flow and solute transport*, Appl. Numer. Math., **61** (2011), pp. 530–553.

[2] J. Fuhrmann, H. Zhao, H. Langmach, Y. Seidel, Z. Jusys, R.-J.Behm, *The role of reactive reaction intermediates in two-step heterogeneous electro-catalytic reactions: A model study*, WIAS Preprint no. 1522, 2010, submitted.

[3] R. Eymard, J. Fuhrmann, A. Linke, *MAC schemes on triangular meshes*, to appear in: Proc. Finite Volumes for Complex Applications, Prague, June 6–10, 2011, Springer.

[4] 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.

[5] 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.

[6] R. Eymard, Th. Gallouët, R. Herbin, A. Linke, *Convergence of a finite volume scheme for the biharmonic problem*, WIAS Preprint no. 1482, 2010, submitted.

[7] A. Bowers, B. Cousins, A. Linke, L. Rebholz, *New connections between finite element formulations of the Navier–Stokes equations*, J. Comp. Phys., **229** (2010), pp. 9020–9025.

[8] O. P. Le Maître, O. M. Knio, *Spectral Methods for Uncertainty Quantification*, Scientific Computation, Springer, Dordrecht [et al.], 2010.

[9] R. Forster, R. Kornhuber, *A polynomial chaos approach to stochastic variational inequalities*, to appear in: J. Numer. Math.

[10] R. Forster, *On the stochastic Richards equation*, Ph.D. Thesis, Freie Universität Berlin, 2011, in preparation.

[11] H. Berninger, *Domain decomposition methods for elliptic problems with jumping nonlinearities and application to the Richards equation*, Ph.D. Thesis, Freie Universität Berlin, Fachbereich Mathematik und Informatik, 2007.

[12] D. Etling, *Theoretische Meteorologie: Eine Einführung*, Springer, Berlin, 2002.

[13] J. Marshall, F. Molteni, *Towards a dynamical understanding of planetary-scale flow regimes*, J. Atm. Sci., **50** (1993), pp. 1792–1818.

[14] CCLM community, *Regional climate modelling with COSMO-CLM CCLM*, Meteorologische Zeitschrift, **17** (2008).

[15] R. Schrodin, E. Heise, *The multi-layer version of the DWD soil model TERRA_ML*, DWD Technical Report **2**, Deutscher Wetterdienst, Offenbach, 2001.

[16] V. Krysanova, F. Wechsung, *SWIM (Soil and Water Integrated Model) user manual*, PIK Report **69**, Potsdam Institute for Climate Impact Research, Potsdam, 2000.

[17] R. Krahl, E. Bänsch, *On the stability of an evaporating liquid surface*, submitted to: Physics of Fluids.

[18] N. Kulev, M. Dreyer, *Drop tower experiments on non-isothermal reorientation of cryogenic liquids*, Microgravity Science and Technology, **22** (2010), pp. 463–474.

[19] E. Fuhrmann, M. Dreyer, *Heat transfer by thermo-capillary convection, sounding rocket COMPERE experiment SOURCE*, Microgravity Science and Technology, **21** (2009), pp. 87–93.

[20] E. Fuhrmann, M. Dreyer, *Description of the sounding rocket experiment — SOURCE*, Microgravity Science and Technology, **20** (2008), pp. 205–212.

[21] E. Bänsch, *Simulation of instationary, incompressible flows*, Acta Math. Univ. Comenian. (N.S.), **67** (1998), pp. 101–114.

[22] *COMPERE: Untersuchung des Treibstoffverhaltens in Raketenoberstufen*, `http://www.dlr.de/rd/desktopdefault.aspx/tabid-2279/3410_read-5108/`.

2.5 Numerical Methods for Population Balance Systems

Sashikumaar Ganesan, Volker John, Ellen Schmeyer, and Carina Suciu

In a general sense, a population is a collection of the same species of individuals that interact with each other. This kind of individuals may be, e.g., solid particles, droplets, or bubbles. Modeling the population by means of a population balance system, one is not interested in the individual species, but in an average behavior of the system.

The studies concentrated so far on population balance systems that model processes from chemical engineering and from physics. These systems consist of equations whose individual numerical simulations are active fields of research, e.g., the incompressible Navier–Stokes equations for turbulent flows and convection-dominated scalar equations. Moreover, the equation for the distribution of the population is defined in a higher-dimensional domain, since the distribution depends not only on time and space but also on properties of the species, the internal coordinates. So far, distributions with one internal coordinate (univariate distributions) have been considered. The main goal is the development of accurate and efficient numerical methods for the simulation of such systems. In addition, the advantages and shortcomings of different approaches for simulating population balance systems are explored.

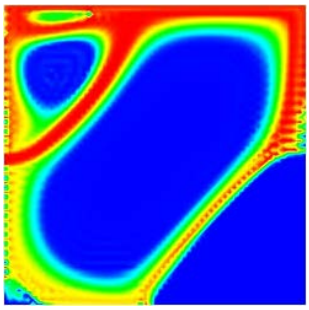


Fig. 1: *Spurious oscillations of a concentration, precipitation process computed with the SUPG method*

Precipitation processes

Precipitation processes are very important in chemical industry. Very well understood from the point of view of chemical engineering is the calcium carbonate precipitation. This process was studied in collaboration with the groups of Prof. K. Sundmacher (Max Planck Institute Magdeburg) and Prof. L. Tobiska (University of Magdeburg).

In a precipitation process, a chemical reaction occurs in a liquid phase. The reactants and the products are dissolved. The main feature of a precipitation process is the nucleation of particles in regions where the local concentration of a product of the chemical reaction, here calcium carbonate, exceeds a saturation concentration. The nucleation of particles and their subsequent growth consume the dissolved product species. Nucleation and growth are the most important mechanisms in precipitation processes. Such processes can be modeled by a coupled system consisting of the Navier–Stokes equations for describing the flow field, convection-diffusion-reaction equations that describe the transport, the reaction and the consumption of dissolved species, and a transport equation for the population of particles, which models their nucleation, growth, and transport. The internal coordinate is the diameter of the particles.

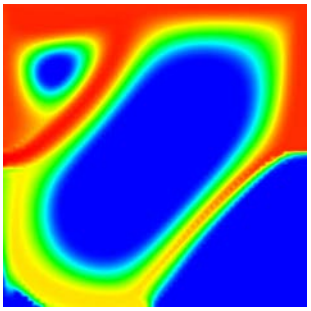


Fig. 2: *Essentially oscillation-free concentration, precipitation process computed with a linear FEM-FCT method*

The simulations of the Navier–Stokes equations and the equations describing the reaction were based on finite element discretizations in space and on implicit time-stepping schemes. For the Navier–Stokes equations, experience has shown that the use of second-order velocity finite element spaces and discontinuous first-order pressure spaces leads to accurate results and efficient simulations. In the case of turbulent flows, a variational multi-scale (VMS) method, which was developed in the group, was applied for turbulence modeling. The convection- and reaction-dominated scalar equations for the dissolved species have to be discretized with a stabilized

method. However, using a standard stabilized finite element method, the streamline upwind Petrov–Galerkin (SUPG) method, led to rather dissatisfactory numerical results; see [5]. Figure 1 shows that with this approach a lot of spurious oscillations occur. Only the application of a completely different approach, finite element flux-corrected transport schemes (FEM-FCT) by Kuzmin et al., could cure this problem; see Figure 2. These schemes have been proven to compute much more physically reliable solutions in comparative studies than a large number of other stabilized finite element methods. The smearing introduced by linear FEM-FCT schemes is in applications more tolerable than spurious oscillations, which correspond to unphysical situations like negative concentrations.

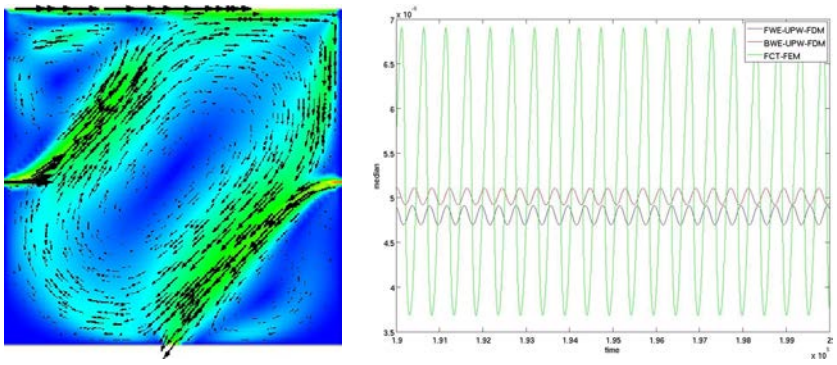


Fig. 3: *Left: laminar flow field. Right: median of the volume fraction for different numerical methods for solving the population balance equation, from [3].*

In addition to the FEM-FCT schemes, also simpler and more inexpensive methods were used for the numerical solution of the equation for the particle size distribution (PSD), namely finite difference simple upwind schemes in combination with the forward (FWE-UPW-FDM) or backward Euler method (BWE-UPW-FDM) as time-stepping scheme. In [3, 4], it could be observed that computed outputs of interest are qualitatively the same if the background flow is laminar; see Figure 3. However, for strongly time-dependent or turbulent flows, large differences in computed outputs of interest occurred, caused by only changing the numerical method for solving the equation for the particle size distribution; see Figure 4. This emphasizes the need for careful studying the effects produced by using different discretizations or even different numerical methods for simulating population balance systems.

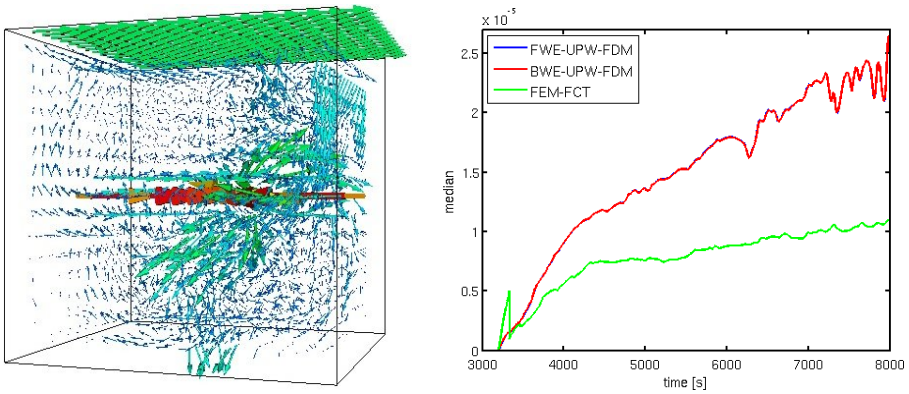


Fig. 4: *Left: turbulent flow field. Right: median of the volume fraction for different numerical methods for solving the population balance equation, the blue and the red curves are on top of each other.*

Numerical studies of academic examples of population balance systems with prescribed solutions show that the results obtained with a linear FEM-FCT scheme are more accurate than with the finite difference upwind schemes. However, the simulations with the latter schemes are considerably faster; compare Table 1.

scheme for solving the PSD equation	16 levels	32 levels	64 levels
forward Euler upwind FDM	19	19	21
backward Euler upwind FDM	19	19	23
Crank–Nicolson FEM-FCT	26	33	64

Table 1: *Precipitation process with 3D turbulent flow, average computing times per time step in* s*, different numbers of levels for discretizing the internal coordinate, from [4]*

Synthesis of urea

The simulation of the synthesis of urea was a project within the BMBF Program *Mathematics for Innovations in Industry and Services* in collaboration with the groups of Prof. W. Hackbusch (Max Planck Institute for Mathematics in the Sciences, Leipzig), Prof. K. Sundmacher (Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg), and Prof. L. Tobiska (University of Magdeburg).

The model of the urea synthesis consists of the Navier–Stokes equations for describing the flow field, scalar convection-diffusion equations for modeling the transport of temperature and of dissolved urea and for modeling their interaction with the urea particles, and finally an equation for the particle size distribution. The coupling of the unknowns in these equations is illustrated in Figure 5. This strong coupling is another reason why discretizations that compute solutions with spurious oscillations are not applicable. Inserting such solutions into other equations might give unphysical coefficients in these equations. This situation easily leads to instable numerical simulations.

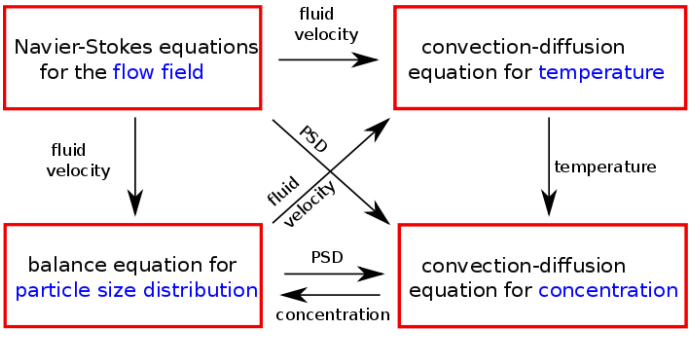


Fig. 5: *Coupling of the unknowns in the simulation of the synthesis of urea*

The main chemical mechanism of the urea synthesis is the aggregation of particles. This process is modeled by integral terms of convolution type in the equation for the particle size distribution, such that this equation becomes an integro-partial differential equation defined in a four-dimensional domain. For the evaluation of these integrals, modern approaches developed in the group of Prof. W. Hackbusch were used. The integral kernel consists of two terms, one models

the aggregation generated by Brownian motion and the other models shear-induced aggregation. Both terms contain unknown parameters that were calibrated on the basis of experimental data provided by the group of Prof. K. Sundmacher. Figure 6 shows representative results of the calibration. Parameters could be identified such that the numerical and experimental data fit quite well.

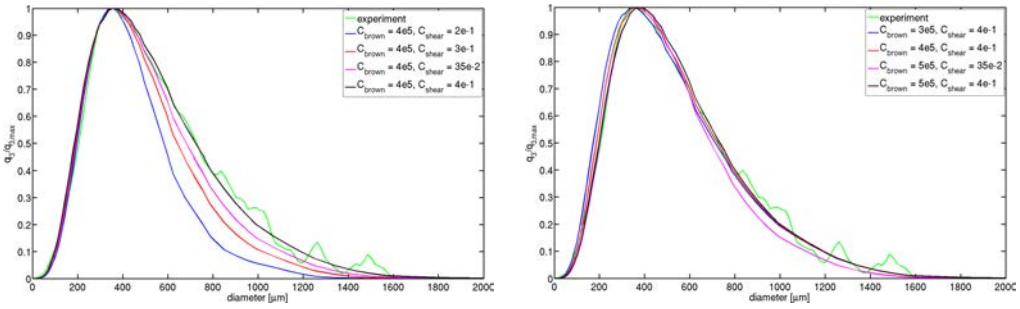


Fig. 6: *Results for the normalized volume fraction obtained with the calibration of model parameters in the simulation of the urea synthesis*

Together with the group of Prof. L. Tobiska, an operator-splitting approach for simulating population balance systems was developed for the example of urea synthesis. Instead of solving the equation for the particle size distribution in the four-dimensional domain, the solution process is split into solving an equation in a one-dimensional domain followed by the solution of an equation in a three-dimensional domain. Compared with the simulation of the equation defined in the four-dimensional domain, this approach is more efficient. However, the splitting technique introduces an additional error. This technique was analyzed in [2]. Its careful comparison with other available approaches is still work in progress.

Droplet size distributions in turbulent flows

Another application studies the distribution of droplets in turbulent flow fields. This is a project within the DFG Priority Program 1276 *MetStröm: Multiple Scales in Fluid Mechanics and Meteorology* in collaboration with the group of Prof. D. Thévenin (University of Magdeburg). A principal goal of this project consists in gathering information on the development of rain droplets in cumulus clouds. Especially, the rapid growth of droplets in the presence of turbulence is an interesting field of research with a lot of open questions.

Data from different wind tunnel experiments are provided by the project partner. A turbulent flow field and the behavior of a droplet size distribution have to be modeled. Up to now, this model includes the growth of droplets in supersaturated air, the transport of droplets in the turbulent flow field and the growth of the droplets caused by aggregation. Similar to the simulation of the urea synthesis, a main aspect is the calibration of model parameters of the aggregation kernel on the basis of experimental data [1]. Since the experimental data are available in discrete points, which are not suited for the application of the methods by the group of Prof. W. Hackbusch, a different approach was developed for the evaluation of the aggregation integrals. This approach is based on approximating certain integrals, which do not depend on the numerical solution, but only on the kernel and the grid for the internal coordinate, in a preprocessing step. The use of preprocessed

data during the simulations results in a rather efficient method. Figure 7 shows a good agreement of the experimental and numerical results for appropriately calibrated parameters.

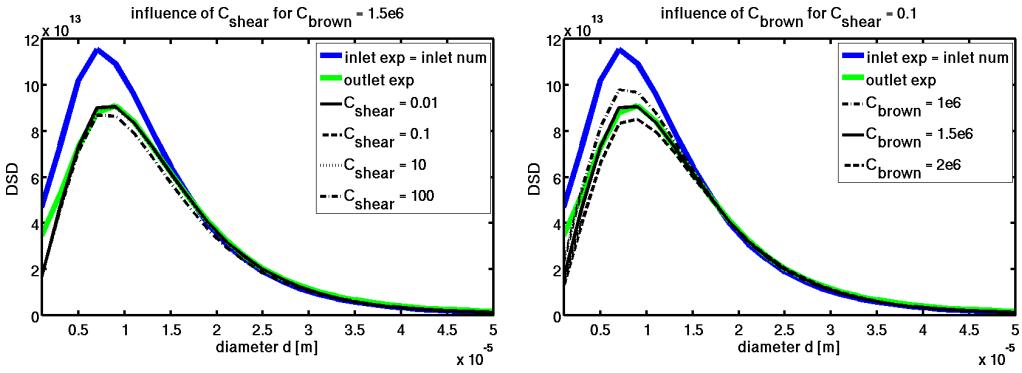


Fig. 7: *Results obtained with the calibration of model parameters in the simulation of a droplet size distribution in a turbulent flow field. The green curve represents the experimental data to compare with.*

Perspectives

The development of accurate and efficient numerical methods for simulating population balance systems is an active field of research. There are many unresolved questions, in particular, concerning the accuracy of the computed results.

Some topics in this field, which will be studied in the near future, are, e.g., the careful comparison of different approaches, multi-variate particle size distributions, the consideration and mathematical study of moment-based methods, and techniques of model order reduction to increase the efficiency of parameter calibration processes.

References

[1] R. Bordás, V. John, E. Schmeyer, D. Thévenin, *Measurement and simulation of a droplet population in a turbulent flow field*, WIAS Preprint no. 1590, 2011, submitted.

[2] S. Ganesan, *An operator-splitting heterogeneous finite element method for population balance equations: Stability and convergence*, WIAS Preprint no. 1531, 2010, submitted.

[3] V. John, M. Roland, *On the impact of the scheme for solving the higher dimensional equation in coupled population balance systems*, Int. J. Numer. Meth. Engng., **82** (2010), pp. 1450–1474.

[4] V. John, M. Roland, *Simulations of 3D/4D precipitation processes in a turbulent flow field*, in: Numerical Mathematics and Advanced Applications, G. Kreiss et al., eds., Springer, Berlin/Heidelberg, 2009, pp. 479–487.

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

2.6 Mathematical Modeling of Entropy-induced Hysteresis

Wolfgang Dreyer and Clemens Guhlke

Hysteresis

Definition of hysteresis. A body that is subjected to a time-dependent load $L : t \in [0, \infty) \to \mathbb{R}$ may respond in two different ways. 1. The response $R : t \in [0, \infty) \to \mathbb{R}$ at time $t = \tau$ of the body is exclusively determined by its load $L(\tau)$ at the same time. 2. The response of the body at time τ depends on the history of the load between $t = 0$ and the actual time τ.

In the latter case, the value $L(\tau)$ does not uniquely determine $R(\tau)$. In particular, if the load assumes its initial value again during the course of time, the value of the response function where this happens is not the corresponding initial value. This phenomenon is called *hysteresis*.

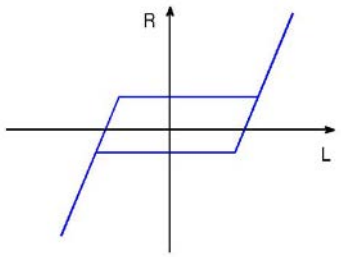


Fig. 1: *Typical load-response diagram exhibiting a hysteresis loop during cyclic loading*

Mathematicians usually restrict their description of hysteresis to processes that are *rate independent*, i.e., they consider only processes where a variation of the loading rate implies the same variation of the rate of the response function. However, in this article we do also consider *rate-dependent* processes.

Physical origins of hysteresis. Hysteresis is a macroscopic phenomenon, but it is related to the microstructure of the body at hand.

The classical occurrence of hysteresis is due to dissipative processes happening on the micro-scale of the body. Among these there is the relative motion of adjacent crystal layers and the migration of point defects or of dislocations. Phenomena of this kind are called *plastic processes*. They are described in two WIAS highlight articles of 2009 [3, 4].

At WIAS, a second kind of hysteresis is treated with applications to lithium-ion batteries, shape-memory alloys, and a system of interconnected rubber balloons. Its origin is essentially different from *plasticity-induced hysteresis*. For differentiation, we introduce the notion *entropy-induced hysteresis* for the latter. Entropy-induced hysteresis occurs under certain conditions in bodies consisting of an ensemble of communicating sub-bodies. Here, hysteresis might even occur if dissipative processes were absent in the sub-bodies. It is due to a cooperative phenomenon of the ensemble, and it is invariably accompanied by a phase transition.

An important example where this happens concerns many-particle electrodes of rechargeable lithium-ion batteries. The ensemble of storage particles exhibits phase transition and entropy-induced hysteresis. These phenomena can be visualized in a system of interconnected rubber balloons, which behaves similarly.

Energy and entropy

The key notions to describe thermodynamic processes are the additive quantities *energy* E and *entropy* S. The evolution of every thermodynamic process is based on a competition between energy and entropy. At high temperature T, a process is controlled by the entropy, whereas the energy is the crucial quantity at low temperature. However, the competition and the emerging evolution of a thermodynamic process to equilibrium is also very much influenced by the boundary conditions.

Energy. If only energy counts, the energy law predicts a strict decrease of energy in a body subjected to proper boundary conditions. In this case, the energy assumes a minimum in equilibrium.

Entropy. If the entropy dominates a thermodynamic process, the entropy law predicts a strict increase of entropy in a body subjected to the same boundary conditions that lead to the minimization of energy in the previous case. Then the entropy assumes a maximum in equilibrium.

Example: Entropy and osmosis. *Osmosis* describes the phenomenon that ground water rises in trees. Here, the tendency to maximize the entropy is more important than the minimization of gravitational energy.

Fig. 2: *Osmosis is a purely entropic effect*

Entropy inequality for isothermal processes. If both energy and entropy control a thermodynamic process, the combination $F \equiv E - TS$, which is called *free energy*, implies the evolution of a body. For isothermal processes and for prescribed load $L(t)$, we have

$$\frac{d(E - TS)}{dt} - \Lambda \frac{dL}{dt} \leq 0\,, \tag{1}$$

where Λ describes the thermodynamic state of the loading and is related to the response function R. For a mechanical load, Λ is the external stress acting on the boundary of the body. In case that the loading consists of the supply of matter, Λ represents the Gibbs free energy of the incoming matter.

Entropy and probability. The statistical definition of the entropy is embodied in a universal formula that reads

$$S = k \log(W)\,. \tag{2}$$

Fig. 3: *The formula that is engraved on Boltzmann's gravestone does not occur in any of his papers*

Here, k is the Boltzmann constant and W is interpreted as the number of *micro states* that may realize a *macro state*. A deep understanding of this vague statement is mandatory to exploit the statistical definition (2). For the purposes of this article, the following example is sufficient:

We consider a game with two dice. A single throw yields a set of two numbers that we call the micro state. A macro state is assumed to be defined by the sum of those numbers. A given macro state can be realized by a distribution of micro states. For example, the macro state 5 can be realized by 4 micro states, thus $W = 4$. Figure 4 self-explains more details.

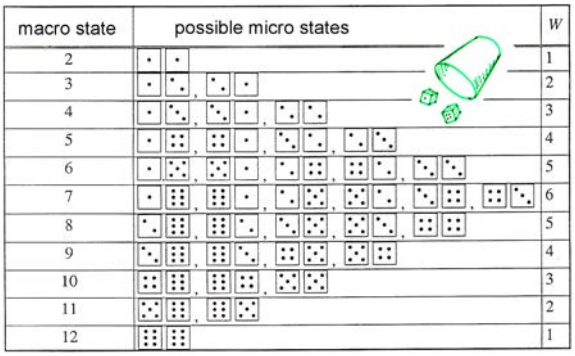


Fig. 4: *Example to illuminate the statistical definition of entropy*

In a physical body, the macro state is given by its thermodynamic state, and the game is generated by thermal fluctuations within the body.

Energy and entropy on the various micro scales. The identification of the possible micro states depends on the chosen *micro scale*, which is not self-evident. Various choices are possible.

For example, on the atomic scale of a body, which is macroscopically described by its volume and energy, the distribution of micro states is formed by the positions and velocities of the atoms. However, entropy-induced hysteresis emerges on a micro scale that is *much more macroscopic*. Here, the micro objects are not atoms but macroscopic systems. We consider in the limit $N \to \infty$ to be an ensemble of N interconnected macroscopic systems whose members are generically called *particles*.

Mathematical model

Micro and macro description. The mathematical model of the ensemble relies on (i) a single statistical variable $\xi \in [a, b]$, which is assigned to each of the N particles, (ii) a free energy $F : [a, b] \to \mathbb{R}$ assigned to each particle, (iii) a nonnegative density $w : t \in [0, \infty) \times [a, b] \to \mathbb{R}_+$ giving the probability that at time t a particle of the ensemble is found in the micro state ξ, and (iv) expressions for the total free energy of the ensemble and of the load that read

$$\mathcal{A}(t) = \int_a^b F(\xi) w(t, \xi) d\xi + kT \int_a^b w(t, \xi) \log(w(t, \xi)) d\xi, \qquad L(t) = \int_a^b G(\xi) w(t, \xi) d\xi\,, \tag{3}$$

where G is some function.

The total free energy $\mathcal{A}$ comprises two different entropic contributions. There is a part that embodies fluctuations on the atomic scale, and that part is included in the individual free energies F of the particles. The second part describes fluctuations in the ensemble and is represented by the second integral of $\mathcal{A}$. That term is a direct consequence of Boltzmann's formula (2).

The evolution law. In this setting, the simplest evolution law for the probability density that identically satisfies the entropy inequality is given by

$$\tau \frac{\partial w(t,\xi)}{\partial t} + \frac{\partial}{\partial \xi}\Big(\big(\Lambda(t)G'(\xi) - F'(\xi)\big)w(t,\xi)\Big) = \nu^2 \frac{\partial^2 w(t,\xi)}{\partial \xi^2}\,. \tag{4}$$

The evolution law is supplemented by an initial condition $w(0,\xi) = w_0(\xi)$ with no-flux boundary conditions at a and b.

The problem is nonlocal because the function $\Lambda(t)$ must be calculated from (3)$_2$. There are two constant parameters: the relaxation time τ of the ensemble and ν^2, which is proportional to kT.

Key technology: Lithium-ion battery

The model will now be applied to a problem of great technical importance: we consider an initial and boundary value problem for a $FePO_4$ many-particle electrode of a modern lithium-ion battery. The electrode is schematically illustrated in Figure 5, which shows an ensemble of nanoparticles on a substrate. The particles serve to reversibly store and release lithium atoms during discharging and charging of the battery.

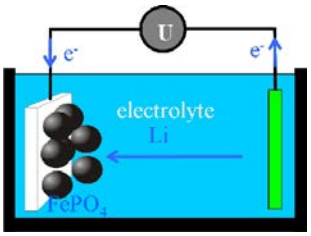


Fig. 5: *Half-cell with many-particle electrode*

The micro scale of that system is controlled by the nanoparticles. A micro state is given by the distribution of stored lithium atoms over the nanoparticles. Thus, the microscopic variable $\xi \in [0,1]$ is identified here as the lithium concentration of a single nanoparticle. The macro state is described by the total loading L, giving the mean concentration of the ensemble. In this case, the generic function G is the identity.

The most important observation during the storage process concerns a phase transition within the ensemble. This phenomenon is mathematically described by a double-well potential F, so that the resulting chemical potential $\mu = F'$ is a non-monotone function of the lithium concentration ξ; see Figure 6.

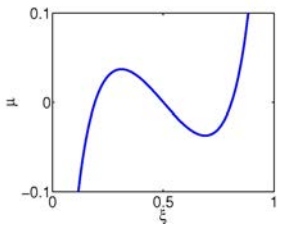


Fig. 6: *Chemical potential*

The response function R of the storage process is chosen here as the voltage of the battery, which is proportional to the mean chemical potential $\langle\mu\rangle = \int_0^1 \mu w\, d\xi$.

We prescribe the history of loading-unloading processes by the load L and solve the evolution equation (4) for the probability density w.

Initially, we start the simulation in the 1-phase region, where the storage particles are Gaussian distributed around a small value, $L_0 = 0.1$; see Figure 7$_{(a)}$. At first, we increase the load L linearly from $L = 0.1$ to $L = 0.9$, and afterwards we decrease it from $L = 0.9$ to $L = 0.1$. The time t has been normalized by $|\dot{L}| = 1$, so the parameter $\tau = \tau_D/\tau_L$ gives the ratio between relaxation

time τ_D of the many-particle system and loading time τ_L. In particular, for fixed τ_D a small τ corresponds to a large loading time.

In order to illustrate the typical behavior of solutions, we choose equal parameters $\tau = \nu^2 = 10^{-4}$. Figure 7 shows snapshots of the probability density at five different times. The arrows indicate the direction of the dynamics.

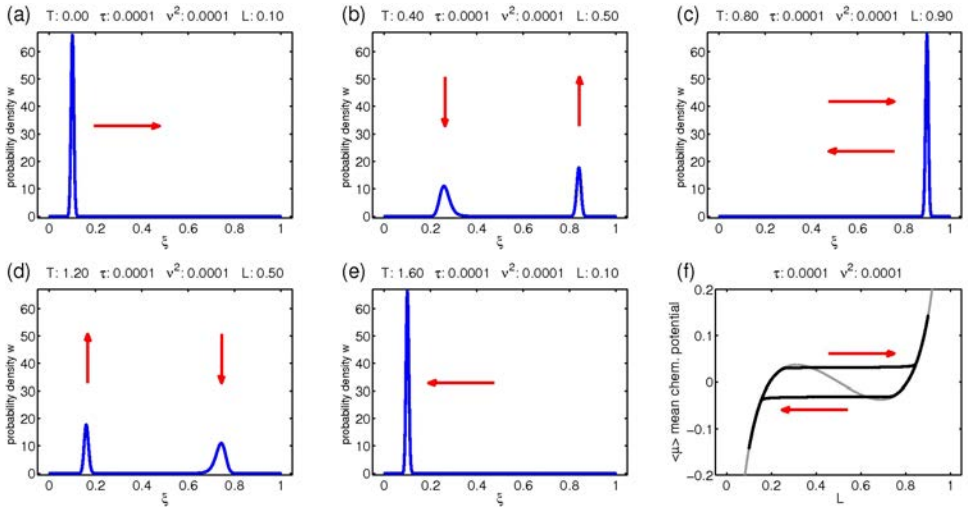


Fig. 7: *(a)–(e): Evolution of the probability density w according a to loading-unloading process for $\tau = 10^{-4}$ and $\nu^2 = 10^{-4}$. (f): $(\langle\mu\rangle, L)$ diagram, black: mean chemical potential $\langle\mu\rangle$, gray: chemical potential of single storage particle μ.*

After a certain period, the initial single pulse decays into two pulses indicating the transition from single phase states to the coexistence region of two phases and back to single phase states for large load L. After L has reached its maximal value, a corresponding dynamics happens the other way around.

It is important to observe that the location where a pulse grows or diminishes is different for the loading and the unloading path. This can be seen by comparing Figures $7_{(b)}$ and $7_{(d)}$, which contain corresponding snapshots for the same load $L = 0.5$. The path dependence of the process becomes clearly manifest by the hysteresis curve in Figure $7_{(f)}$. It contains the $(\langle\mu\rangle, L)$ diagram and reveals how the mean chemical potential $\langle\mu\rangle$ depends on the load L.

References

[1] W. Dreyer, J. Jamnik, C. Guhlke, R. Huth, J. Moškon, M. Gaberšček, *The thermodynamic origin of hysteresis in insertion batteries*, Nature Materials, **9** (2010), pp. 448–453.

[2] W. Dreyer, C. Guhlke, M. Herrmann , *Hysteresis and phase transition in many-particle storage systems*, Contin. Mech. Thermodyn., **23(3)** (2011), pp. 211–231.

[3] S. Heinz, A. Mielke, A. Petrov , *Mathematical modeling of hysteresis and plasticity in materials with microstructures*, Annual Research Report 2009, WIAS, Berlin, pp. 39–43.

[4] D. Knees , *Progress in the regularity theory for elasto-plasticity*, Annual Research Report 2009, WIAS, Berlin, pp. 44–48.

2.7 A New Level of Reliability for Phase Field Simulations

Rüdiger Müller

The phase field method is commonly accepted as a versatile and stable numerical method for the analysis and prediction of microstructures. As these microstructures strongly influence material properties, their understanding is of great importance in modern production technology. They are not a fixed material property but evolve over time. Phase separation and coarsening lead to aging of materials and favor the initiation of cracks along phase boundaries that might finally lead to failure of a device.

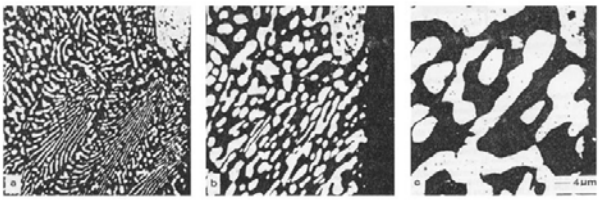


Fig. 1: *Coarsening of the microstructure in a binary SnPb solder alloy at* $125\,^{\circ}\mathrm{C}$. *Micrographs taken immediately after solidification (a), after* $3\,h$ *(b) and after* $300\,h$ *(c).*

Moving phase boundaries that undergo topological changes are very difficult to track computationally. Phase field methods are used to regularize the interface motion problem by smearing out sharp interfaces into fronts of finite width $\gamma > 0$; see Figure 2. Already with very few degrees of freedom in the interface, it is possible to compute numerical solutions that look convincing but might be misleading and suggest wrong temporal or spacial scales. To approximate the sharp interface limit $\gamma \to 0$ accurately, grid adaption methods are needed that concentrate degrees of freedom at the interface regions. This requires an a posteriori error control but, unfortunately, conventional error estimates depend exponentially on γ^{-1} and hence become useless if $\gamma \ll 1$.

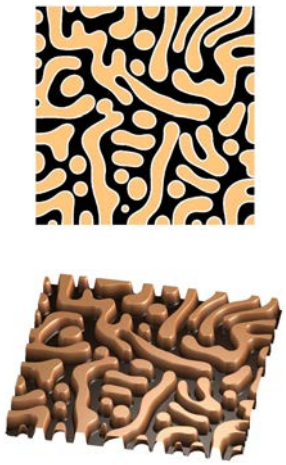


Fig. 2: *Bulk phases separated by sharp interfaces and a phase field representation of the same situation*

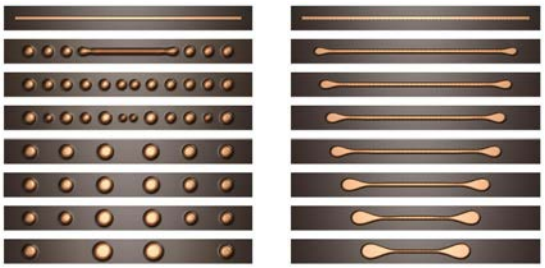
The numerical analysis of phase field methods is well established for fixed interface parameter size $\gamma > 0$, cf. [3], but until recently, it has only been insufficiently developed for the approximation of the sharp interface limit. The achievements of this research project are to have established computable a posteriori error estimates for phase field equations of Allen–Cahn, Ginzburg–Landau and Cahn–Hilliard type that are robust with respect to $\gamma \to 0$ and

1. hold beyond topological changes of the diffuse interfaces,
2. do not impose restrictive conditions on the initial values,
3. are valid for singular logarithmic potential functions.

This theoretical foundation is necessary to justify the phase field method as a reliable prediction technique but has not been available before. Moreover, the involved error estimators provide in a natural way local grid refinement and coarsening indicators that are required for the practical simulation of realistic scenarios.

The numerical solution responds very sensibly to topological changes in the phase field. Realistic simulations of microstructures contain many of these topological changes where small fluctuations may lead to a very different overall solution; see Figure 3. The techniques presented here

allow to detect critical points in the evolution and thereby measure the stability of the problem and the reliability of the simulation.



$\gamma = 1/32$ $\gamma = 1/96$

Fig. 3: *Cahn–Hilliard evolution of a bar-shaped particle: for $\gamma = 1/32$, the simulation shows "temporary negative coarsening" (left); this phenomenon is an artefact of the phase field method that vanishes as $\gamma \to 0$ (right)*

The Cahn–Hilliard model

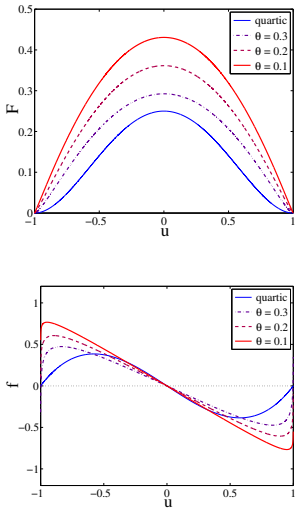


Fig. 4: *Free energy contribution F and $f = F'$ for different temperatures and the quartic approximation*

Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, be a Lipschitz domain. Phase field models are based on the minimization of an energy functional of the form $\mathcal{E}(u) = \int_\Omega \frac{\gamma}{2}|\nabla u|^2 + \frac{1}{\gamma} F(u)\,dx$. Here, F represents the free energy contribution. For binary alloys, F has a double-well structure, and its two minima correspond to the two phases. For temperatures θ close to the transition temperature θ_c, polynomial growth of F, e.g. $F(u) = (u^2 - 1)^2/4$, provides a good description, whereas in other situations it is necessary to take a logarithmic growth of F into account, i.e.,

$$F(u) = \frac{\theta}{2}\big[(1+u)\ln(1+u) + (1-u)\ln(1-u)\big] - \frac{\theta_c}{2}u^2\,. \tag{1}$$

More generally, the free energy is required to satisfy certain growth conditions:

Assumption. *Let $0 < \theta < \theta_c$. There is a splitting of the form $F(u) = \theta\phi(u) + \theta_c\psi(u)$, where $\phi \in C^4$ is a smooth convex function, and $\psi \in C^2$ satisfies some cubic growth condition on the derivative ψ'.*

$0 < \theta \le \theta_c$, and $\mathcal{I} = (-1, 1)$. There exists a convex smooth function $\phi \in C^4(\mathcal{I})$ satisfying $\phi'', \phi^{(4)} \ge 0$ in $\mathcal{I}$, and $\psi \in C^2(\mathcal{I})$ such that $F = \theta\phi + \theta_c\psi$ in $\mathcal{I}$ and

$$(\psi'(a) - \psi'(b))(a-b) \ge \psi''(a)(a-b)^2 - g(a)|a-b|^3$$

for all $a, b \in \mathcal{I}$ with a nonnegative function $g \in C(\mathcal{I})$.

The Cahn–Hilliard equation is derived by taking the H^{-1} gradient flow of the energy $\mathcal{E}$, leading to the fourth order nonlinear parabolic equation

$$\partial_t u - \Delta\big(\gamma^{-1} f(u) - \gamma\,\Delta u\big) = 0\,. \tag{2}$$

The mathematical model is closed by prescribing suitable initial and boundary conditions such that existence of a unique weak solution is guaranteed. Here, natural boundary conditions are considered, i. e., no boundary contributions enter into a weak formulation of (2). For the initial data, some weak spatial differentiability is required, leading to a setting in the Sobolev space $H^1(\Omega)$.

Allen–Cahn– and Ginzburg–Landau equations can also be derived from the same energy functional $\mathcal{E}$ and additional effects like elastic deformations can be included by introducing more terms to $\mathcal{E}$. In each of these cases it was possible to achieve results analogous to those presented below [1, 2].

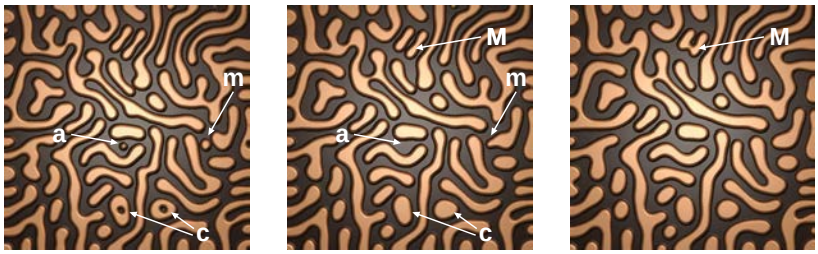


Fig. 5: *Simulation of coarsening by Cahn–Hilliard evolution. $\theta = 0.2$ and $\gamma = 1/64$ on the domain $\Omega = (-2, 2)2$. Different topological changes of the solution between the snapshots are marked (a = absorption of a particle, c = closing of voids, m,M = merging of particles)*

Abstract a posteriori error analysis

In a finite element simulation, we choose at each time level $t_j \in [0, T]$ a shape regular triangulation of Ω. Then we seek a discrete solution u_h^j in a finite-dimensional subspace of $H^1(\Omega)$. Let $\|\cdot\|$ denote the L^2 norm over Ω, and by u_h we denote the piecewise affine interpolation of u_h^j with respect to time. Let u be the weak solution to (2) and u_h a finite element function obtained by some numerical scheme. The *error* is defined as $e := u_h - u$ and satisfies the differential equation

$$\frac{1}{2}\frac{d}{dt}\|\nabla\Delta^{-1}e\|^2 + \gamma\|\nabla e\|^2 = -\gamma^{-1}(f(u_h) - f(u), e) + \langle\mathcal{R}_1, \Delta^{-1}e\rangle + \langle\mathcal{R}_2, e\rangle\,, \tag{3}$$

where $\mathcal{R}_1$ and $\mathcal{R}_2$ denote *residual* terms that are obtained as remainder when inserting the numerical solution u_h into a mixed weak form of (2).

The abstract a posteriori analysis requires no assumptions on how the approximate solution was obtained. A suitable numerical scheme was given in [1], together with fully computable *residual estimators* μ_{-1}, μ_0, μ_1 such that

$$\langle\mathcal{R}_1(t), \zeta\rangle + \langle\mathcal{R}_2(t), \chi\rangle \le \mu_{-1}(t)\|\nabla\zeta\| + \mu_0(t)\|\chi\| + \mu_1(t)\|\nabla\chi\|$$

for almost every $t \in [0, T]$ and all test functions ζ, χ. For different numerical schemes, such estimators can be derived by standard techniques.

To bound the error, information about the stability properties of the Cahn–Hilliard operator was needed. The sensitivity of the numerical solution to possible amplification of errors is characterized by the *principal eigenvalue* λ_{CH} of the linearized operator

$$-\lambda_{\mathrm{CH}}(t) := \inf_{q\in V\setminus\{0\}} \frac{\gamma\|\nabla q\|^2 + \gamma^{-1}\big(f'(u(t))q, q\big)}{\|\nabla\Delta^{-1}q\|^2}\,, \tag{4}$$

where V is the subspace of functions in $H^1(\Omega)$ having mean value 0. With these ingredients, it was possible to derive from (3) the inequality

$$\frac{1}{2}\frac{d}{dt}\|\nabla\Delta^{-1}e(t)\|^2 + \frac{\gamma^4}{2}\|\nabla e\|^2 \le \eta^2 + 2\alpha(s)\|\nabla\Delta^{-1}e\|^2 + \frac{2}{\gamma}B(t)\|e\|^3_{L^3(\Omega)}\,,$$

with a computable quantity $B(t)$ that depends on $f(u_h)$ and an estimator η that is composed of μ_{-1}, μ_0, μ_1 and $\alpha(t) = \big(2\theta_c^2 \sup_{x\in\Omega} |\psi''(u_h(t,x))|^2 + \lambda_{\mathrm{CH}}(t) + 1\big)$. To prove an abstract error estimate, the term containing $\|e\|^3_{L^3(\Omega)}$ required the application of a generalized Gronwall lemma that led to a smallness condition for the residuals.

Theorem (Bartels and Müller 2010).
If $\int_0^T \eta^2(s)\,\mathrm{d}s + \|\nabla\Delta^{-1}e(0)\|^2 \le C\,\exp\big(-3\int_0^T \alpha(s)\,\mathrm{d}s\big)\big(\sup_{s\in[0,T]} B(s)\big)^{-2}(1+T)^{-2}$, then

$$\sup_{s\in[0,T]} \|\nabla\Delta^{-1}e(s)\|^2 + \frac{\gamma^4}{2}\int_0^T \|\nabla e\|^2\,\mathrm{d}s \le 8\Big(\int_0^T \eta^2(s)\,\mathrm{d}s + \|\nabla\Delta^{-1}e(0)\|^2\Big)\cdot\exp\Big(2\int_0^T \alpha^+(s)\,\mathrm{d}s\Big). \tag{5}$$

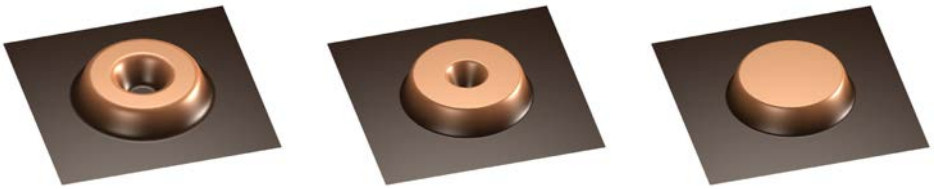


Fig. 6: *Snapshots of the simulation of a prototypical topological change related to case (c) in Figure 5*

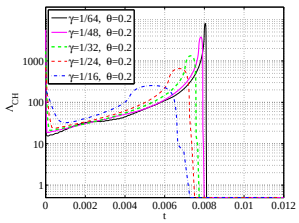


Fig. 7: *Evolution of the principal eigenvalue $\lambda_{\mathrm{CH}}(t)$ in the simulation illustrated in Figure 6*

Robust error control beyond topological changes

In the above theorem, there is no explicit exponential dependence on γ^{-1}, but the right-hand side contains the principal eigenvalue $\lambda_{\mathrm{CH}}(t)$. Starting with [5], robust a priori and a posteriori error estimates for Allen–Cahn and the Cahn–Hilliard equations have been developed that were based on uniform bounds for λ_{CH} given in [4]. These bounds require that the phase field represents smooth profiles across interfaces, leading to restrictive assumptions on the initial data. Moreover they break down when topological changes occur; see Figure 7. In general, these singularities cannot be predicted in advance and, hence, it is not possible to determine the range where these estimates are valid. For Cahn–Hilliard equations with elasticity or other, more complicated situations, no such uniform spectral estimate is available so far.

A slightly different approach was taken here, where we followed the philosophy to "replace as much analytical knowledge as possible with computational knowledge". By linearizing the Cahn–Hilliard operator at the approximate solution $u_h(t)$ instead of $u(t)$, and numerically computing the principal eigenvalue λ_{CH}, it is possible to determine critical times where previously available error estimates break down, and we are able to assess the stability of the simulated phase field model.

The necessary a posteriori and a priori error estimates for the numerical solution of the eigenvalue problem have been derived in [1].

Numerical experiments revealed that topological changes for which $\lambda_{\mathrm{CH}}(t) \sim \gamma^{-3}$ occur within temporal intervals of length comparable to γ^3. As can be seen in Figure 8, this leads to a logarithmic bound of the form

$$\int_0^T \max(0, \lambda_{\mathrm{CH}}(s))\,ds \le C + \ln \gamma^{-\kappa}. \tag{6}$$

Replacing previous L^∞ bounds on λ_{CH} by an L^1-norm estimate according to (6), a novel a posteriori error control has been derived that is robust even beyond finitely many topological changes

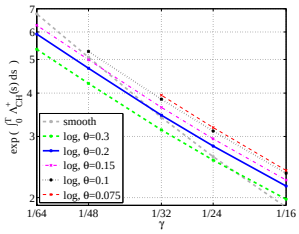


Fig. 8: *Time-integrated eigenvalue over the interface parameter γ for different temperatures θ*

in the solution, rather than just allowing the detection of these singularities.

Proposition. *If (6) holds and* $\int_0^T \eta^2(s)\,\mathrm{d}s + \|\nabla\Delta^{-1}e(0)\|^2 \le C\,\gamma^{\kappa}\left(\sup_{s\in[0,T]} B(s)\right)^{-2}(1+T)^{-2}$, *then*

$$\sup_{s\in[0,T]} \|\nabla\Delta^{-1}e(s)\|^2 + \frac{\gamma^4}{2}\int_0^T \|\nabla e\|^2\,\mathrm{d}s \le C\,\gamma^{-3\kappa}\cdot\left(\int_0^T \eta^2(s)\,\mathrm{d}s + \|\nabla\Delta^{-1}e(0)\|^2\right). \qquad (7)$$

Numerical experiments also show that initial perturbations of an interface relax sufficiently fast to be compatible with the bound (6) for time-integrated eigenvalue λ_{CH}. In this way, the restrictions on the initial data are removed.

Figure 9 shows the time evolution of $\lambda_{\mathrm{CH}}(t)$ in the situation of an initially bar-shaped particle illustrated in Figure 3. As γ is reduced, the peaks that indicate the topological changes grow in height, but since there are far less of these singularities for $\gamma = 1/48$, the time-integrated eigenvalue that enters the error estimate is lower in this case. For $\gamma = 1/96$, there are no topological changes at all. We can conclude that, as γ is reduced, the Cahn–Hilliard evolution of the bar-shaped particle becomes more stable and the simulation results become a more reliable approximation of the sharp interface limit.

In the deep quench limit $\theta = 0$, the logarithmic potential has to be replaced by a nonsmooth obstacle potential leading to a problem of variational inequalities. The numerical experiments indicate convergence of λ_{CH} as $\theta \to 0$, see Figure 8. Although the formulation of the corresponding linearization and its principal eigenvalue is not obvious, it seams reasonable to expect the possibility of robust error control also in the case of the obstacle potential.

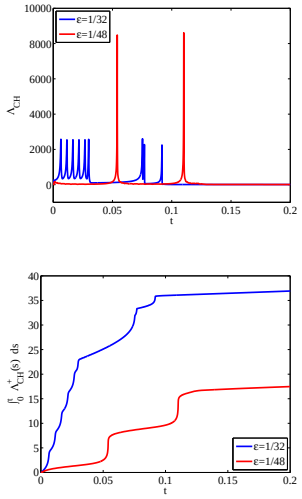


Fig. 9: *Evolution of* $\lambda_{\mathrm{CH}}(t)$ *and the time-integrated eigenvalue for the evolution of a bar-shaped particle according to Figure 3*

References

[1] S. Bartels, R. Müller, *Error controlled local resolution of evolving interfaces for generalized Cahn–Hilliard equations*, Interfaces Free Bound., **12(1)** (2010), pp. 45–73.

[2] S. Bartels, R. Müller, *Error control for the approximation of Allen–Cahn and Cahn–Hilliard equations with a logarithmic potential*, WIAS Preprint no. 1539, 2010, submitted.

[3] M.I.M. Copetti, C.M. Elliott, *Numerical analysis of the Cahn–Hilliard equation with a logarithmic free energy*, Numer. Math., **63(1)** (1992), pp. 39–65.

[4] X. Chen, *Spectrum for the Allen–Cahn, Cahn–Hilliard, and phase-field equations for generic interfaces*, Comm. Partial Diff. Eqs., **19(7-8)** (1994), pp. 1371–1395.

[5] X. Feng, A. Prohl, *Numerical analysis of the Allen–Cahn equation and approximation for mean curvature flows*, *Numer. Math.*, **94(1)** (2003), pp. 33–65.

2.8 Optimal control with pdelib

Klaus Krumbiegel and Timo Streckenbach

Fig. 1: *Partial electron beam hardening of camshafts (pro-beam AG & Co.KGaA)*

The software environment pdelib provides a framework to integrate numerical algorithms for partial differential equations (PDEs), including mesh generation, numerical solution, and visualization. It is used in a number of applied projects within WIAS, e.g., electron beam hardening of steel. The user interface is designed to minimize the training period for new users, especially for those who are more familiar with *Matlab*. The paradigm is to minimize the inhibition threshold of potential users by an easy-to-use operator-based structure, while maintaining the efficiency and functionality of a C++ code. In the case of optimal control problems driven by PDEs, this concept has proven to be very powerful. The operator-based structure allows for a block-wise assembly of vector and matrix values on cell, face, and node domains, which opens the possibility to handle PDE systems in a flexible manner.

Linear-quadratic elliptic optimal control problems

In the following, a simple model problem is considered illustrating the structure of PDE-constrained optimal control problems and thus the challenges related to an efficient implementation of numerical algorithms treating such problems:

$$\begin{aligned} \min \quad J(y,u) &:= \frac{1}{2}\|y - y_d\|^2_{L^2(\Omega)} + \frac{\nu}{2}\|u\|^2_{L^2(\Omega)}, \\ -\Delta y &= u \qquad \text{in } \Omega, \\ y &= 0 \qquad \text{on } \partial\Omega. \end{aligned}$$

A possible physical background for the PDE in this optimal control problem is the stationary temperature distribution in a solid body occupying the domain Ω. The optimal control problem yields an optimally distributed heat source u such that the difference between the associated temperature distribution y and a desired state y_d is minimal.

The existence of a unique optimal control with associated state for the above problem can be proven by standard arguments; see, e.g., [4]. By introducing a Lagrange multiplier with respect to the state equation, necessary and sufficient optimality conditions can be established; see (1) below. This Lagrange multiplier p is often called *adjoint state* and represents the solution to a respective adjoint equation,

$$\begin{aligned} -\Delta \bar{y} &= \bar{u} \quad \text{in } \Omega, & -\Delta \bar{p} &= \bar{y} - y_d \quad \text{in } \Omega, \\ \bar{y} &= 0 \quad \text{on } \partial\Omega, & \bar{p} &= 0 \qquad \text{on } \partial\Omega, \\ & & \bar{p} + \nu\bar{u} &= 0 \quad \text{in } \Omega. \end{aligned} \tag{1}$$

The optimality system can be written as a linear system of equations where the symmetric system

matrix exhibits the so-called *saddle point structure*

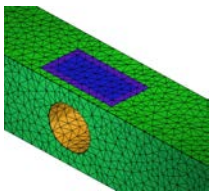
$$\begin{pmatrix} \nu I & 0 & I \\ 0 & I & \Delta \\ I & \Delta & 0 \end{pmatrix} \begin{pmatrix} \bar{u} \\ \bar{y} \\ \bar{p} \end{pmatrix} = \begin{pmatrix} 0 \\ y_d \\ 0 \end{pmatrix}. \tag{2}$$

In order to prepare a numerical simulation, a mesh generator subdivides the workpiece domain Ω into a finite number of subdomains. For each of these so-called *finite elements*, the unknown variables are approximated using higher-order polynomials. The resulting finite element method (FEM) is the standard method in numerical approximation of PDEs over complicated domains.

This method is used to approximate the state and the adjoint state of the optimality system (1). The control can be discretized by means of piecewise constant or piecewise linear ansatz functions.

All of the following code lines are written in the syntax of the extension language Lua [1], which provides a script-based interface to the underlying pdelib C++ application programming interface. One of the primary benefits of scripting is flexibility during runtime of a program, e.g., changing data and top-level program logic. The following few lines generate the mesh shown below, select a suitable finite element type that defines local functions of polynomial order p, and create a finite element function space:

```
grid = gRead("slot_profile.grid")
elem = etFindH1Simplex(gGridDim(grid),p)
space = gsCreate(grid,elem)
```



Based on this finite element function space, suitable operators are defined to discretize the entries in the above linear system (2):

```
K  ≈  Δ     K = feOperator("Int_gradU_gradV_dc", "one", desc)
M  ≈  I     M = feOperator("Int_U_V_dc", "one" , desc)
yd ≈  y_d   yd = feOperator("Int_F_V_dc", "yd", desc)
```

In terms of finite element analysis, K relates to a stiffness matrix, M to a mass matrix, and yd to a state vector. However, these so-defined values are not matrices and vectors, but rather the rules to generate them. The matrix of the linear system (2) and the vectors are initialized by

```
blocksize = 3
KKT = feMatrix0(space,blocksize,solver) -- 3 x 3 block sparse matrix
X = feVector0(space,blocksize) -- solution vector for u, y, p
F = feVector0(space,blocksize) -- right-hand side
```

These lines allocate the necessary memory and select an appropriate solver for the respective linear system of equations. Then, the finite-dimensional counterpart of the linear system (2) is assembled into the matrix and vector structures by combining the previously defined rules:

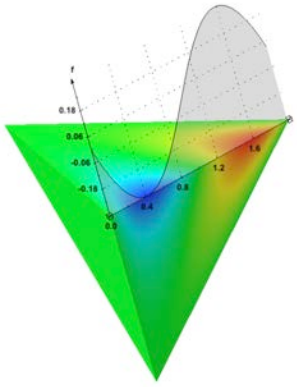


Fig. 2: *Finite element edge function of polynomial order* $p = 3$

$$\underbrace{\begin{pmatrix} \nu M & 0 & M \\ 0 & M & K \\ M & K & 0 \end{pmatrix}}_{\texttt{KKT}} \underbrace{\begin{pmatrix} \bar{u} \\ \bar{y} \\ \bar{p} \end{pmatrix}}_{\texttt{X}} = \underbrace{\begin{pmatrix} 0 \\ y_d \\ 0 \end{pmatrix}}_{\texttt{F}}$$

```
feMatrixAdd(KKT,
  {{   M*nu    ,     0    ,   M   },
   {     0     ,     M    ,   K   },
   {     M     ,     K    ,   0   }}, desc)
feVectorAdd(F,
   {     0     ,    yd    ,   0   }, desc)
```

In a last step, the linear system is solved by the chosen solver, and the discrete optimal control `u` and the associated state `y` are extracted from the solution vector `X`:

```
feSolve(KKT, X, F, desc)
u = feVectorGet(X, feBlock_i(1))
y = feVectorGet(X, feBlock_i(2))
```

This example illustrates the level at which a user can specify an optimal control problem in `pdelib`. At a similar level, more involved and practically relevant problems can be handled, as described in the next two sections.

Optimal control in electron beam shaping

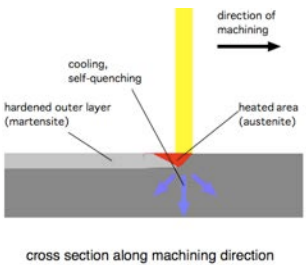


Fig. 3: *Electron beam hardening of steel*

In this section, an optimal control problem is considered that describes the electron beam surface hardening of steel, a process that becomes more and more important, especially in automotive industry. Its mode of operation is depicted in Figure 3. An electron beam moves along the surface of a workpiece, creating a heated zone around its trace. The heating process is accompanied by a phase transition, which produces the high-temperature phase in steel, called *austenite*. Since the penetration depth of the electron beam is very small, the heated zone of the workpiece is rapidly quenched by self-cooling due to heat exchange with the surrounding material. Rapid cooling invokes a further phase transition, which transforms austenite into martensite, a hard and brittle steel phase.

The optimal control of this process is modeled by a so-called *linear-quadratic elliptic boundary control problem*. Neglecting the phase transitions, it takes the form

$$\begin{aligned} \min \quad J(y,u) := \frac{1}{2}\|y - y_d\|^2_{L^2(\Sigma)} + \frac{\nu}{2}\|u\|^2_{L^2(\partial\Omega_1)}, & \\ -\nabla\cdot(\kappa\nabla y) = f \qquad & \text{in } \Omega, \\ \partial_n y = u \qquad & \text{on } \partial\Omega_1, \\ \partial_n y = 0 \qquad & \text{on } \partial\Omega_2, \\ y = y_g \qquad & \text{on } \partial\Omega_3, \\ u_a \le u \le u_b \qquad & \text{on } \partial\Omega_1, \\ y \le y_c \qquad & \text{in } \Sigma. \end{aligned} \tag{3}$$

In various applications of PDE-constrained optimization, additional inequality constraints regarding the control or the state are necessary. In the case of the above problem, additional control constraints allow to incorporate threshold values for the electron beam power. Moreover, pointwise state constraints, such as $y(x) \leq y_c(x)$ a.e. in Σ, prevent the melting of the considered solid body. In the case of additional inequality constraints, the optimality system of an optimal solution can no longer be written as a linear system. In particular, for control constraints $u \in U_{ad}$, the equation $\bar{p} + \nu\bar{u} = 0$ in (1) has to be replaced by a so-called *variational inequality*. A very efficient optimization algorithm for solving such problems is the *primal-dual active set strategy*. A detailed description of the algorithm can be found in [2].

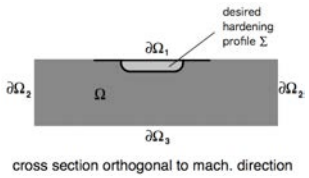


Fig. 4: *Workpiece across machine direction*

The treatment of additional pointwise state constraints is more involved, since Lagrange multipliers regarding these constraints are in general no proper functions, but only measures. However, appropriate regularization techniques allow for the application of the same efficient optimization methods as in the control-constrained case; see [3] and the references therein.

The aim of the optimal control problem introduced above is to achieve a preferably uniform temperature distribution of 800 K in the subdomain Σ, i.e., we choose $y_d = 800$. Furthermore, the state constraints were given by $y \leq 900$ K. Figure 5 illustrates that the optimal temperature distribution is rather uniform and close to the desired state. Besides that, the optimal electron beam power at the boundary part $\partial\Omega_1$ is shown.

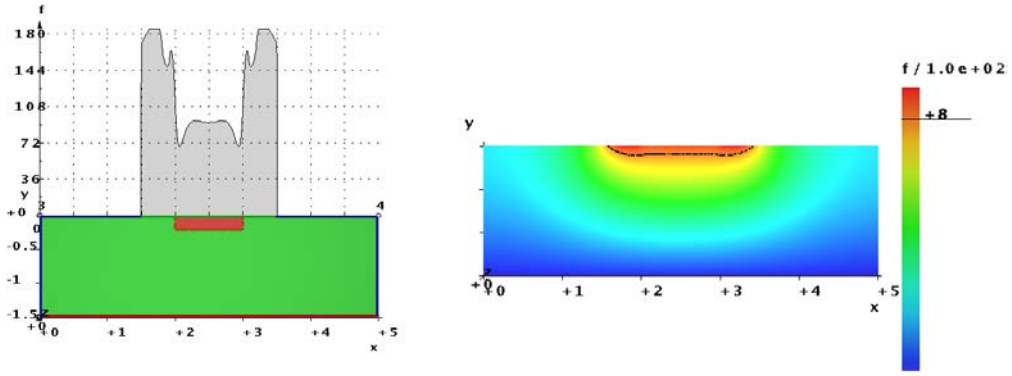


Fig. 5: *Numerical results with state constraints: optimal electron beam power (left), optimal temperature distribution (right)*

Adaptivity based on goal-oriented estimates. The mesh of the domain Ω may be uniform and relatively fine, or it may be adapted to the evolving process, based on so-called *goal-oriented error estimates* [5]. Roughly, the idea is to introduce a simulation goal, here the quantity of interest is the value of the cost functional $J(y, u)$, and estimate an error distribution concerning this measure. Local error estimators indicate where a refinement is necessary in order to guarantee that the overall error is smaller than a given threshold. This method leads to a significant reduction of the number of unknowns in the linear system compared to a uniform mesh refinement, and therefore it saves computational time and memory. Figure 6 shows the results for a three-dimensional version of problem (3), obtained by adaptive mesh refinement based on goal-oriented estimates. Due to the particular structure of the cost functional $J(y, u)$, the refinement is mainly restricted to the desired domain Σ; see Figure 6 a).

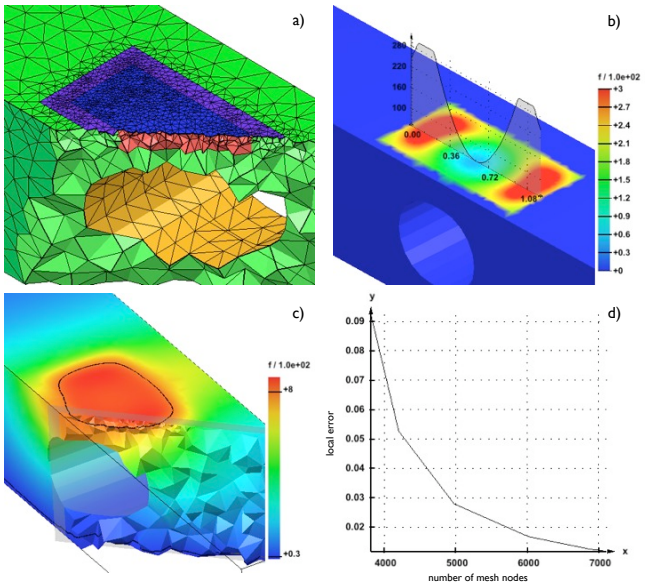


Fig. 6: *Numerical results: a) adapted mesh, b) optimal electron beam power, c) temperature profile, and d) reduction of local error during adaptive steps*

Perspectives

Future work will mainly focus on extending the `pdelib` toolbox in order to cover a wider range of optimal control problems. In particular, iterative solvers and preconditioners for the KKT-system matrices have to be implemented for three-dimensional problems. Moreover, the simulation of parabolic optimal control problems will be enabled. The extension of the built-in operator library with higher-order edge element discretization of Maxwell equations is also work in progress.

References

[1] R. Ierusalimschy, *Programming in Lua*, Second Edition, Lua.org, Rio de Janeiro, 2006.

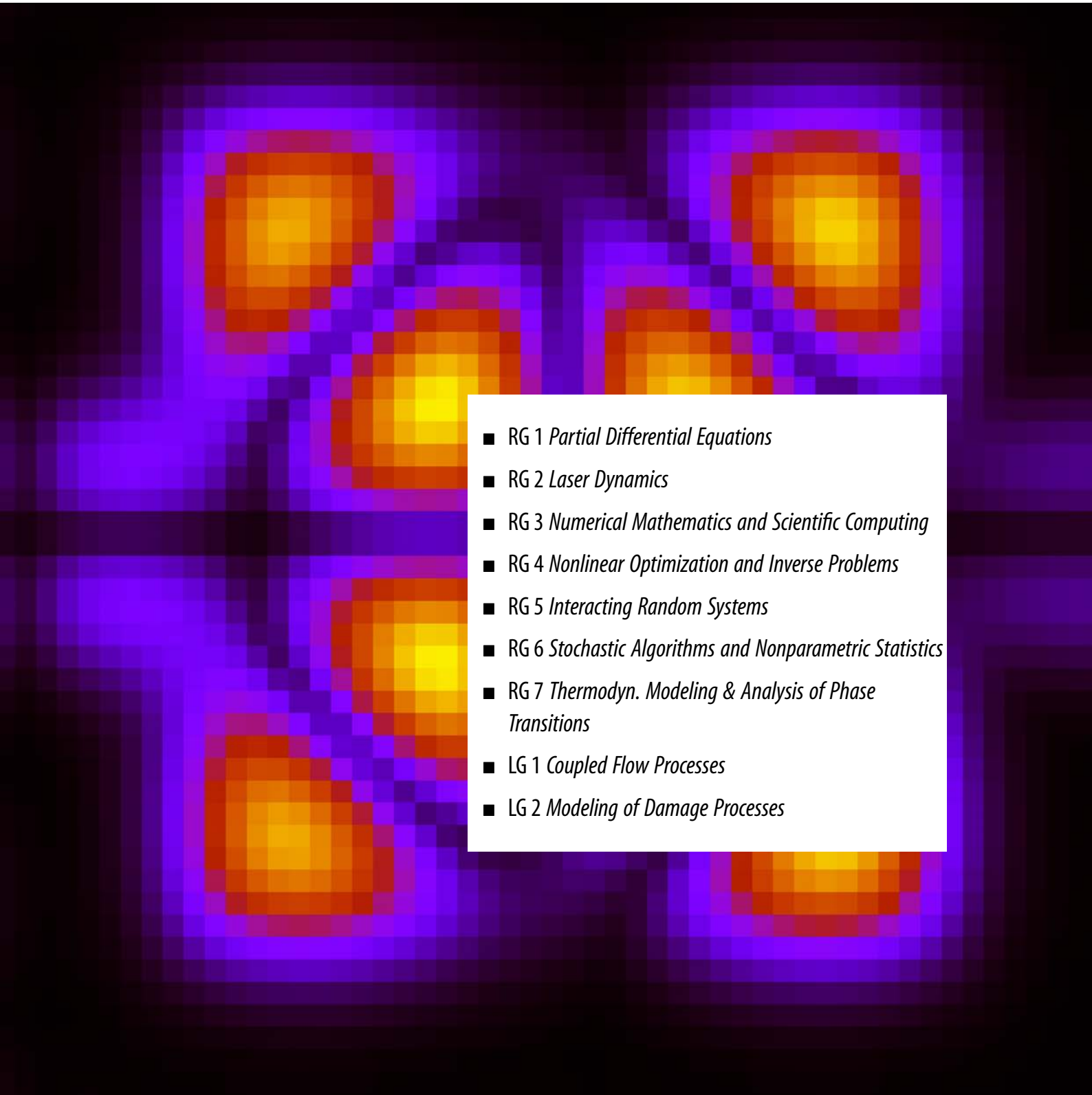
[2] M. Bergounioux, K. Ito, K. Kunisch, *Primal-dual strategy for constrained optimal control problems*, SIAM J. Control Optim., **37** (1999), pp. 1176–1194.

[3] K. Krumbiegel, C. Meyer, A. Rösch, *A priori error analysis for linear quadratic elliptic Neumann boundary control problems with control and state constraints*, SIAM J. Control Optim., **48** (2010), pp. 5108–5142.

[4] P. Neittaanmäki, J. Sprekels, D. Tiba, *Optimization of Elliptic Systems. Theory and Applications*, Springer Monographs in Mathematics, Springer, New York, 2006.

[5] W. Bangerth, R. Rannacher, *Adaptive Finite Element Methods for Differential Equations*, Lectures in Mathematics, ETH Zürich, Birkhäuser, Basel, 2003.

3 Research 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 *Thermodyn. Modeling & 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.

Regularity theory for partial differential equations. During the last years, there has been a growing necessity to investigate parabolic equations with nonsmooth data: bad domains, discontinuous coefficients, and mixed boundary conditions. For example, this investigation is required for optimal control problems studied jointly with the Research Group *Nonlinear Optimization and Inverse Problems*. For homogeneous Neumann boundary conditions, parabolic equations can be solved in the usual space $L^p(\Omega)$; if they are inhomogeneous, the scale of $H^{-\theta,q}$ spaces turns out to be adequate—even for nonlinear equations. This approach has the disadvantage that indicator functions are not admissible test functions and, thus, Gauss's theorem is not available. Hence, one is not in the position to establish local balances for the flux vectors, which are crucial for a rigorous foundation of numerical procedures, e.g., in semiconductor theory.

Following a suggestion of Gröger, it was possible to show that the spaces $L^p(\Omega \cup \Gamma, dx + d\sigma)$ are suitable for the treatment of parabolic equations with inhomogeneous Neumann (or Robin) conditions— Γ being the Neumann boundary part, dx the Lebesgue measure on the domain Ω, and $d\sigma$ the induced surface measure on Γ. In detail, it was proved via a theorem of Cialdea/Maz'ya that elliptic divergence operators of second order generate contraction semigroups on the above-mentioned spaces $L^p(\Omega \cup \Gamma, dx + d\sigma)$. Then, a deep result of Lamberton yields maximal parabolic regularity for such operators. This is achieved here for the highly nonsmooth constellations mentioned above, thereby improving similar approaches from the literature.

Material modeling. The research in this area is devoted to the mathematical modeling and the analysis of elastic solids with additional properties. The focus lies on features that can be described via internal variables with a quasi-static evolution. This research includes damage and crack propagation, which are investigated in collaboration with the Leibniz Group *Modeling of Damage Processes* (LG 2), as well as elastoplastic deformations and phase transformations in shape memory alloys.

The MATHEON project C18 "Analysis and numerics of multidimensional models for elastic phase transformations in shape memory alloys" is concerned with a three-dimensional model of thermally-induced phase transformations in shape memory alloys, for which error estimates for space-time discretizations are obtained; see [4].

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" started its second period on October 1, 2010. In the same month, the European Research Council announced that Alexander Mielke's research proposal "Analysis of Multiscale Systems Driven by Functionals" was successful and receives an *Advanced Research Grant* for the period 2011–2015.

In February 2010, Marita Thomas finished her Ph.D. studies within the DFG Research Training Group 1128 "Analysis, Numerics and Optimization of Multiphase Problems" at the Humboldt-Universität zu Berlin. In her Ph.D. thesis entitled "Rate-independent damage processes in nonlinearly elastic materials", she studied the existence of energetic solutions to a model for partial, isotropic damage and analyzed their temporal regularity. Moreover, using the theory of Γ-convergence for rate-independent systems, it was shown that models describing the partial damage of three-specimen-sandwich structures with vanishing thickness $2\varepsilon \to 0$ of the middle component approximate a delamination model, which includes transmission as well as unilateral contact conditions and which reflects Griffith's fracture criterion; see Figure 1 and [5]. The results on the temporal regularity were also published in the review article [3] in cooperation with Dorothee Knees (LG 2).

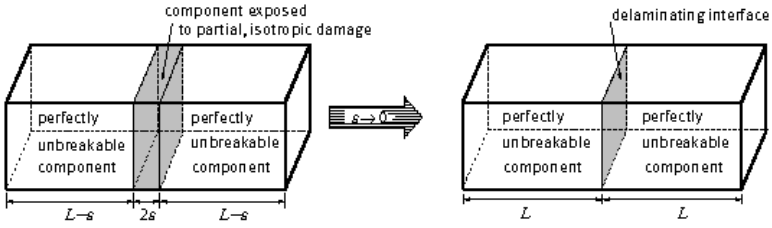


Fig. 1: *Limit passage from damage to delamination*

On March 14–20, 2010, the Workshop "Mircostructures in Solids: From Quantum Models to Continua", organized by Alexander Mielke and Michael Ortiz (California Institute of Technology), took place at the Mathematisches Forschungsinstitut Oberwolfach. It brought together 50 mathematicians and applied scientists and enabled them to discuss the relevant physical effects and their pertinence for the understanding of materials as well as the mathematical methods modeling the formation of microstructures and the effective description of small-scale effects on larger scales. The stimulating discussion between the different research communities created many interesting links between previously disconnected research topics.

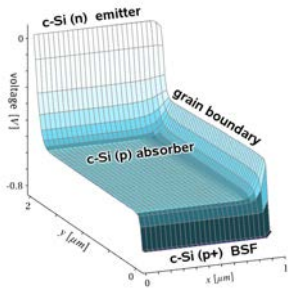


Fig. 2: *Electrostatic potential in a polysilicon solar cell*

Photovoltaics. In 2010, the new MATHEON project D22 "Modeling of electronic properties of interfaces in solar cells" started with the aim to find adequate models for the electronic behavior of solar cells including interface kinetics. It is planned to investigate their analytical properties, to derive suitable numerical approximations, and to provide simulation results, which can be used for calibration with experiments of the Institute for Silicon Photovoltaics at the Helmholtz Centre Berlin for Materials and Energy (HZB). After an accurate comparison of `WIAS-TeSCA` simulations with the one-dimensional photovoltaics simulation tool AFORS-HET of HZB, higher-dimensional problems were tackled; see Figure 2. Moreover, in collaboration with the Institute for Heterogeneous Materials Systems at HZB, the research group continued the two-dimensional and three-dimensional simulations for a novel concept of $CuInS_2$ chalcopyrite-based thin-film heterojunction cells with a point contact/defect passivation structure at the heterointerface; see Figure 3.

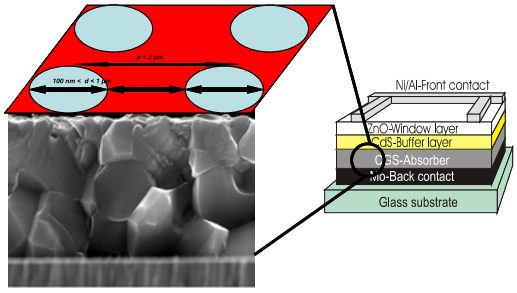


Fig. 3: *Point contacts in passivation layers for an enhanced performance of thin-film solar cells based on wider band gap chalcopyrites*

As an industrial cooperation in photovoltaics, a research and development project with ODERSUN AG is running. It is devoted to the "Modeling and simulation of $CuInS_2$ thin-film solar cells on Cu-tape (CISuT) and module structures".

First analytical results on electronic models for solar cells including energy-resolved defect densities were obtained in [1]. The thermodynamic correctness of the model was verified, a priori estimates of solutions were established, and existence and uniqueness of weak solutions was shown. Methods developed in [2] allow for assertions concerning steady states of such problems. The next important challenges are the modeling and analytical treatment of active interfaces.

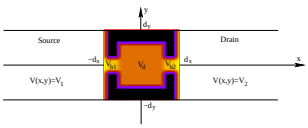


Fig. 4: *Sketch of a single-electron transistor*

Resonance theory for single electron transistors. The functionality of modern semiconductor nano-optoelectronic devices inherently bases on quantum effects like tunneling and the formation of resonances. Therefore, their precise description is essential for the improvement and design of semiconductor devices. The resonances occur at specific energy levels that depend on the geometry and the material parameters of the quantum system. The macroscopic properties, such as the current-voltage diagram, can be derived via a scattering theory for the associated Schrödinger operator. A resonance theory was developed that is based on the R-matrix formalism describing the interaction between resonances in two- or three-dimensional quantum systems [6]. A so-called *single-electron transistor* was studied, which is a quantum dot isolated in a two-dimensional electron gas by two quantum point contacts; see Figure 4. The resonances appear as peaks with different profiles in the linear conductance of the single-electron transistor; see Figure 5. There, one can see a configuration of interacting resonances, which qualitatively describes the experimental data in the Fano regime of transport [J. Göres et al, Phys. Rev. B 62, 2188 (2000)]. There are resonant

states similar to the eigenstates of the isolated dot, see Figure 6, and hybrid resonant states. Similar to the hybrid atomic orbitals, the hybrid resonant states are obtained as a linear combination of degenerate eigenstates with the same parity.

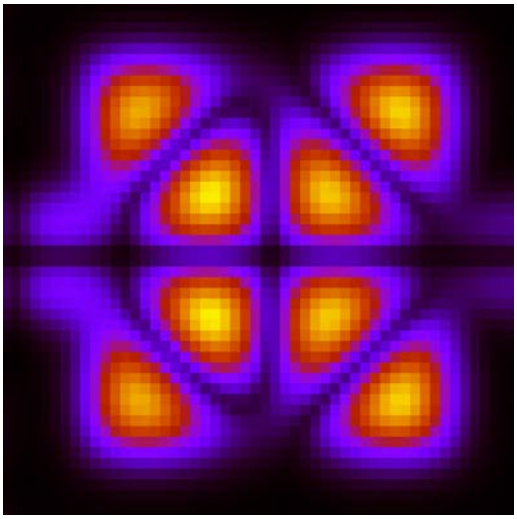


Fig. 5: *Conductance as a function of the potential energy in the dot region. The maps represent the electron probability distribution density* $|\psi_n^{(s)}(E_F; x, y)|^2$ *inside the dot for* $V_d = V_0^{(n_x,n_y)}$ *(vertical dashed lines), for which the resonance energy equals the Fermi energy* $E_0^{(n_x,n_y)} \simeq E_F$*; the pairs of resonances* $(2,4)$ *&* $(4,2)$ *and* $(4,1)$ *&* $(3,3)$ *yield hybrid resonant modes.*

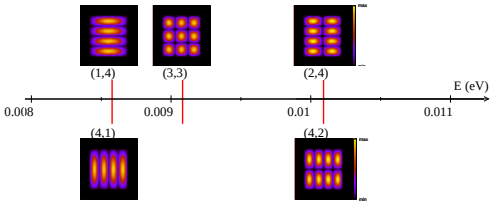


Fig. 6: *The eigenenergies* $\tilde{E}_{n_x,n_y}$ *and the densities* $|\tilde{\psi}_{n_x,n_y}(x, y)|^2$ *of the eigenstates* ψ_{n_x,n_y} *for the isolated dot. Bright and dark regions correspond to high and low densities, resp.*

Kohn–Sham density functional theory (DFT) for semiconductor devices. On July 2, 2010, Kurt Hoke defended his dissertation entitled "Iteration acceleration for the Kohn–Sham system of DFT for semiconductor devices" at the Technische Universität Berlin. DFT-based calculations were succesfully used for electronic-structure simulation of confined semiconductor heterostructures. The Kohn–Sham system determines the densities of multi-particle systems, e.g., of electron and holes, via a nonlinearly coupled system of Schrödinger equations for all eigenstates and the Poisson equation for the electrostatic potential. Apart from the latter and the heterostructure potential, various exchange-correlation effects were also included according to the configuration of the device. Based upon the results concerning existence, uniqueness (in special cases), and regularity of solutions of such multi-particle equilibrium Kohn–Sham systems, an iterative numerical procedure for their solution was implemented using a finite-volume discretization scheme. The crucial point was to overcome convergence problems of the iterative procedure caused by non-convex exchange-correlation energies. So, iteration acceleration for the Kohn–Sham system was investigated together with Reinhold Schneider (TU Berlin). A Kohn–Sham system of the sketched kind is a nonlinearly coupled system of PDEs on a bounded, generically non-smooth domain (due to the

device geometry) with mixed boundary conditions and jumping coefficients (due to the heterostructure). The challenge of these non-smooth constellations could be overcome by the regularity theory for second-order elliptic divergence operators developed recently in this research group.

International Conferences

6th Singular Days on Asymptotic Methods for PDEs. This workshop took place at WIAS from April 29 through May 1, 2010, and was partially supported by DFG. It was organized by Annegret Glitzky (RG 1) and Dorothee Knees (LG 2) who were supported by the international scientific board consisting of Martin Costabel (Rennes), Monique Dauge (Rennes), Serge Nicaise (Valenciennes), and Anna-Margarete Sändig (Stuttgart). Besides three key-note presentations, there took place 21 talks and a poster session. The main topics were regularity results for elliptic and parabolic PDEs on nonsmooth domains or with nonsmooth coefficients, suitably adapted numerical methods and applications from physics and mechanics.

International Symposium on Trends in Applications of Mathematics to Mechanics. The 17th STAMM took place in Schmöckwitz from August 30 through September 2, 2010, was jointly organized by WIAS and Wolfgang Müller, TU Berlin, and was attended by about fifty engineers, mathematicians, and physicists. This bi-annual conference series is devoted to current topics in applied mathematics and mechanics. This year, there was a special emphasis on self-organized criticality in fracture, damage, and plasticity as well as on the mechanics of active materials and on the matching of micro- and nanoscales. On September 1, a *Special Ericksen Session* was held in the honor of the first awardee Jerry L. Ericksen of the newly established *ISIMM Prize*, which is awarded for outstanding achievements in promoting the interaction between mathematics and mechancis.

In memoriam Arno Langenbach

Arno Langenbach, the founder of the Berlin Seminar on Nonlinear Partial Differential Equations, passed away at the age of 81 on February 11, 2010. Berlin's scientific community lost an outstanding mathematician and mentor; his scientific legacy and enthusiasm will always be treasured.

References

[1] A. Glitzky, *Analysis of electronic models for solar cells including energy resolved defect densities*, WIAS Preprint no. 1524, 2010, to appear in: Math. Methods Appl. Sci.

[2] A. Glitzky, K. Gärtner, *Existence of bounded steady state solutions to spin-polarized drift-diffusion systems*, SIAM J. Math. Anal., **41** (2010), pp. 2489–2513.

[3] P. Gruber, D. Knees, S. Nesenenko, M. Thomas, *Analytical and numerical aspects of time-dependent problems with internal variables*, ZAMM Z. Angew. Math. Mech., **90** (2010), pp. 861–902.

[4] A. Mielke, L. Paoli, A. Petrov, U. Stefanelli, *Error estimates for space-time discretizations of a rate-independent variational inequality*, SIAM J. Numer. Anal., **48** (2010), pp. 1625–1646.

[5] A. Mielke, T. Roubíček, M. Thomas, *From damage to delamination in nonlinearly elastic materials at small strains*, WIAS Preprint no. 1542, 2010, submitted.

[6] E.R. Racec, U. Wulf, P.N. Racec, *Fano regime of transport through open quantum dots*, Phys. Rev. B, **82** (2010), pp. 085313/1–085313/16.

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 2010 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 "Localized Structures in Dissipative Nonlinear Systems", October 18–20, organized by the research group at WIAS. The workshop brought together researchers from all over the world working in the field of theoretical and experimental studies of nonlinear systems exhibiting self-organized dissipative structures. Particular attention was paid to spatial and temporal localized structures — so-called *optical dissipative solitons*. A review article about this topic has been coauthored by Shalva Amiranashvili; see Figure 1. An important success for the group's research was the continuation of the DFG Research Center MATHEON, where the group will continue the projects D8 and D14 (see page 110). The group members expanded their teaching activities through a special lecture at the Humboldt-Universität Berlin (HU), in addition to their two traditional research seminars "Mathematical Photonics" and "Nonlinear Dynamics", organized together with HU and the Freie Universität Berlin (FU), respectively. Uwe Bandelow became a Privatdozent at HU Berlin and was a member of the Program Committee of NUSOD for its 2010 conference in Atlanta, USA.

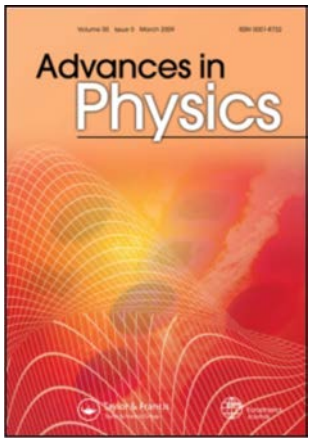


Fig. 1: *In this journal, in vol.* **59** *(2010), pp. 485–701, the review article* Dissipative solitons *by H.-G. Purwins, H. U. Bödeker, and Sh. Amiranashvili was published*

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

Dynamics of semiconductor lasers

The recently developed theoretical approach for delay-differential equations with large delay was applied to the Lang–Kobayashi system for lasers with long-delayed optical feedback [2]. In this way, a complete description of the stability properties of all external cavity modes in the limit of large delay could be given. In particular, this approach enabled to distinguish between different types of weak and strong instabilities and to calculate bifurcation diagrams that indicate the transitions between them.

The effect of carrier exchange between the wetting layer and discrete energy states in quantum dot lasers on their dynamical properties was studied numerically using delay differential equations and traveling wave (TWE) models [4], where corresponding carrier exchange rate equations were implemented. To account for Coulomb effects in quantum dot (QD) lasers, also precomputed look-up tables for carrier-carrier scattering rates were introduced into the group's software package `LDSL-tool` . These models were applied to study the operation regimes of QD mode-locked lasers. It was shown that the behavior of these lasers strongly depends on the relative length of the gain and absorber sections. When the absorber section is relatively long, a bistability arises between the zero intensity state and mode-locking regimes (see left panel in Figure 2). The undesired Q-switching instability, leading to a drastic increase in the pulse amplitude noise, is completely eliminated in this case. By contrast, for short absorber length, in addition to usual Q-switched

mode-locking, the existence of a small domain of pure Q-switching (see right panel in Figure 2) was predicted theoretically and confirmed later in experiments.

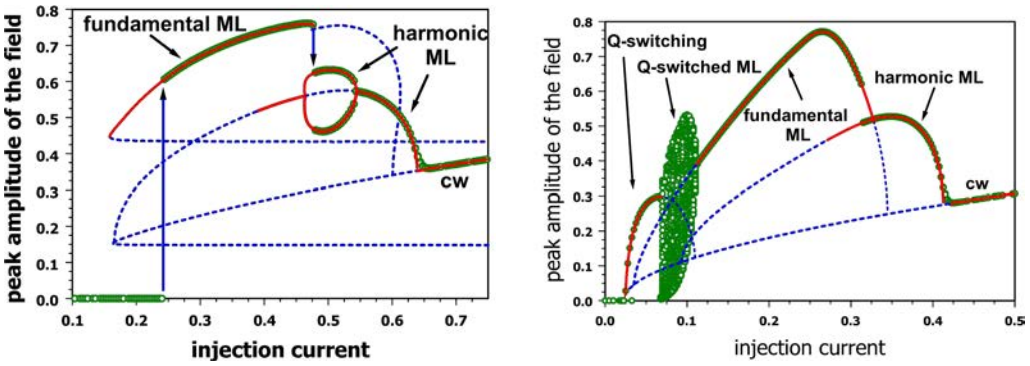


Fig. 2: *Bifurcation diagram illustrating the transition of different dynamical regimes in a mode-locked quantum dot laser with increasing injection current. Stable (unstable) solutions are shown by solid (dotted) lines. The gray dots correspond to the extrema of the absolute value of the electric field amplitude obtained by means of direct numerical simulations. Left: long absorber section. Right: short absorber section.*

Hybrid mode-locking in a monolithic QD laser was studied using the delay differential model, and a strong asymmetry of the locking range was found. This asymmetry, similar to that observed experimentally by partners from the SFB 787 in TU Berlin, was interpreted as a manifestation of a nonlinear resonance phenomenon. The group's model explains the appearance of the locked state as a result of saddle-node and inverse Andronov–Hopf bifurcations at small and large modulations of the reverse bias applied to the absorber section, respectively. An asymptotic analysis for the dependence of the locking range on the parameters was performed on small reverse bias modulation amplitudes. An equation governing the slow time evolution of the phase difference between mode-locked solution and external modulation was derived, and the coefficient for the ratio between the size of the locking range and the reverse bias modulation amplitude was calculated. The results of the theoretical analysis suggest an improved device operation by incorporation of a spectral filtering element into the cavity.

The group's activities in modeling, simulation, and analysis of tapered and broad area lasers, based on a 2D extension of the TWE model, were also continued in 2010. In particular, design rules for the Bragg gratings were derived from these simulations. Numerical results on the output characteristics of edge-emitting distributed Bragg reflector tapered lasers agreed well with the experimental results from the group's partners at the Ferdinand Braun Institute for High-Frequency Technology, Berlin. The analysis enabled to explain and to estimate the spectral behavior and the periodic reoccurrence of dynamic instabilities. Wavelength stabilization in distributed-feedback master-oscillator power amplifiers emitting optical powers of several watts with high brilliance was calculated. In addition, striped array lasers operating under angular feedback were studied.
A fully finite difference scheme approximating this model for broad area lasers was shown to provide a speed-up by a factor of two. The error induced by the approximation of the discrete transparent lateral boundary conditions and the convergence of the numerical solutions were studied in particular as well as the adaption of the numerical mesh to the laser geometry.

Pulses in nonlinear optical media

The propagation of ultrashort optical pulses in a non-absorbing nonlinear dispersive medium was considered from the Hamiltonian point of view. To this end, first a second-order nonlinear wave equation for the electric field was exactly transformed into a first-order propagation equation for a suitably defined complex electric field. The governing equation involves a proper rational approximation to the medium dispersion function. Positive and negative frequency parts of the complex electric field correspond to forward and backward waves, respectively. For the unidirectional pulse propagation, the complex field contains only positive harmonics and reduces to the analytic signal. In a second step, the Hamiltonian framework was introduced for the complex formulation in terms of two classical fields referring to quantum creation and annihilation operators. The derived z-propagated Hamiltonian accounts for forward and backward waves, arbitrary medium dispersion, and four-wave mixing processes. The Hamiltonian approach was applied for the derivation of integrals of motion for the pulse propagation. These integrals were demonstrated to reflect time-averaged fluxes of energy, momentum, and classical photon number transferred by the pulse. The conserved quantities can be used to control the numerics and to classify solitary solutions to the underlying equations [1].

Within a joint DFG project on pulse shaping in hollow-fiber compressors with experimental partners from the Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin, filamentary self-compression of optical pulses in a gaseous medium was investigated as an alternative to traditional pulse compression schemes. The latter utilize the (focusing) Kerr effect in guiding structures that can be described by nonlinear Schrödinger-type equations. However, in filamentary self-compression, an additional equation has to account for the generation of a defocusing plasma. These effects yield a strongly time-dependent beam waist, leading to a temporal pulse breakup; see Figure 3. Ultimately, the process results in an ultrashort on-axis temporal pulse profile. It turns out that laser pulses resulting from this cascaded self-compression scenario exhibit characteristic spatio-spectral signatures. During this project, the theoretical predictions were confirmed in experimental investigations.

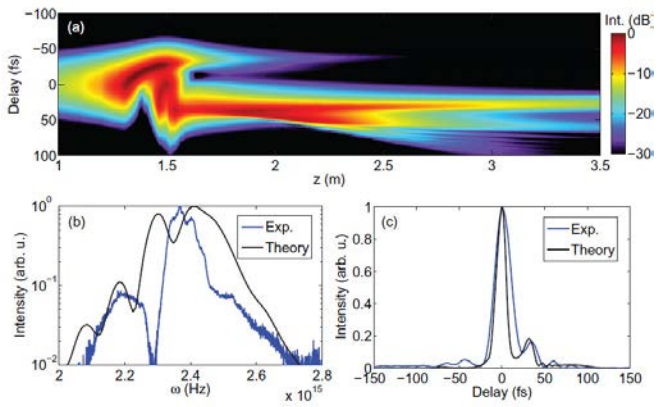


Fig. 3: *(a) Evolution of on-axis temporal intensity along z in a numerically simulated filament in air, exhibiting refocusing stage and double splitting events. (b) On-axis spectra in numerical simulation and experiment. (c) On-axis temporal intensity profile from SPIDER measurement (blue curve) versus on-axis profile at $z = 3.5$ m obtained from numerical simulations (black curve).*

In a new project on *Vacuum ultraviolet and terahertz pulse generation in bulk media and guided ge-*

ometries based on plasma generating femtosecond light pulses within the DFG Individual Grants Program, a comprehensive model was developed, allowing to simulate the process of THz generation in a plasma generated by strong asymmetric optical fields in noble gases. Several basic setups were studied, such as plasma spots created by tight focusing of input beams and hollow metallic capillary [6], where simulation results agreed excellently with experiments. The results in [6] allowed to confirm that the key mechanism responsible for the THz generation is indeed the low-frequency part of the radiation emitted by the photoinduced plasma current. The importance of certain pulse propagation effects, such as frequency blue shift and spatio-temporal reshaping of the pump, was demonstrated [6].

Further research on pulse propagation focused on supercontinuum generation in a ring resonator, performed in a collaborative project with the University of Rostock (Prof. F. Mitschke).

Dynamical systems

A recent focus in this field was the investigation of complex dynamics in large coupled systems. For recent results on chimera states, see the Scientific Highlights article *Chimera States: Spatiotemporal Patterns of Synchrony and Disorder* on page 20. In [3], the emergence of high-dimensional chaos in a ring of coupled nonlinear oscillators was described. Here, the coupling induces a transition from stable equilibrium to periodically rotating waves, chaos, and hyperchaos. This research was carried out in a new bilateral cooperation with the National Academy of Sciences of Ukraine, funded by German Research Foundation.

The properties of 2D dissipative structures of light in a coherently driven optical resonator subjected to a delayed feedback were investigated in [5]. The phenomenon of spontaneous motion of these structures induced by the feedback was studied in detail. In particular, it was shown that the delayed feedback induces a spontaneous motion of periodic patterns and dark localized structures. An optical bistability regime was analyzed, where the space-time dynamics was described by a variational Swift–Hohenberg equation. In the absence of delayed feedback, dark localized structures and patterns do not move. This behavior occurs only when the product of the delay time and the feedback strength exceeds some critical value.

References

[1] Sh. Amiranashvili, A. Demircan, *Hamiltonian structure of propagation equations for ultrashort optical pulses*, Phys. Rev. A, **82** (2010), pp. 013812/1–013812/11.

[2] M. Wolfrum, S. Yanchuk, *A multiple timescale approach to the stability of external cavity modes in the Lang–Kobayashi system using the limit of large delay*, SIAM J. Appl. Dyn. Syst., **9** (2010), pp. 519–535.

[3] P. Perlikowski, S. Yanchuk, M. Wolfrum, A. Stefanski, P. Mosiolek, T. Kapitaniak, *Routes to complex dynamics in a ring of unidirectionally coupled systems*, Chaos, **20** (2010), pp. 013111/1–013111/9.

[4] A. G. Vladimirov, U. Bandelow, G. Fiol, D. Arsenijević, M. Kleinert, D. Bimberg, A. Pimenov, D. Rachinskii, *Dynamical regimes in a monolithic passively mode-locked quantum dot laser*, J. Opt. Soc. Amer. B Opt. Phys., **27** (2010), pp. 2102–2109.

[5] M. Tlidi, A. G. Vladimirov, D. Turaev, G. Kozyreff, D. Pieroux, T. Erneux, *Spontaneous motion of localized structures and localized patterns induced by delayed feedback*, Eur. Phys. J. D, **59** (2010), pp. 59–65.

[6] I. Babushkin, W. Kuehn, Ch. Köhler, S. Skupin, L. Bergé, K. Reimann, M. Woerner, J. Herrmann, Th. Elsaesser, *Ultrafast spatio-temporal dynamics of terahertz generation by ionizing two-color femtosecond pulses in gases*, Phys. Rev. Lett., **105** (2010), pp. 053903/1–053903/4.

3.3 Research Group 3 "Numerical Mathematics and Scientific Computing"

The research group focuses on the development of numerical methods, their numerical analysis, and the implementation of software tools for the numerical solution of partial differential equations and differential-algebraic systems. Most of these developments are performed in the context of applications. In this way, an impact of the developed methods is given on other fields of research and on industrial partners.

A very close collaboration existed with the Leibniz Group *Coupled Flow Processes in Energy and Environmental Research* (LG 1). In accordance with the suggestions of the commission that evaluated WIAS in 2010, the research of LG1 will be continued within this research group, thus extending its research fields by the topic of modeling and simulation of electrochemical systems.

Additional collaborations exist with the Research Groups *Partial Differential Equations* (RG 1) and *Laser Dynamics* (RG 2) in the field of modeling, analysis, and simulation of charge transport in semiconductor devices. Numerical methods and software tools for optimal control in thermomechanical problems are developed together with the Research Group *Nonlinear Optimization and Inverse Problems* (RG 4).

A short overview will be given of the main topics of the group's research. Further information can be found in the Scientific Highlight articles on pages 43 and 58.

The Voronoi finite volume method

In three space dimensions, the Voronoi box based finite volume method on boundary-conforming Delaunay meshes [1] combines meshing and discretization techniques in such a way that the discrete maximum principle and the positivity of numerical solutions of convection-diffusion problems are guaranteed. Straightforward and economic extensions to systems of equations are possible.

In close cooperation with RG 1, LG 1, and the Leibniz Group *Modeling of Damage Processes*, the group continued to develop numerical simulation approaches based on this method. This work includes contributions to the analysis of the method [4, 7] and the investigation of discretization schemes for the Navier–Stokes equations. A necessary prerequisite for the application of the method are algorithms for the creation of boundary-conforming Delaunay meshes as they are developed in the `TetGen` project. The method is utilized for semiconductor device simulation projects and, together with LG 1, for simulations of reaction processes in electrochemical flow cells.

Mesh generation with `TetGen`

For the generation of three-dimensional boundary-conforming Delaunay meshes, the software tool `TetGen` has been developed. The focus on these meshes originated from the requirements of

the Voronoi box based finite volume scheme. TetGen also has various applications in areas such as visualization, computer-aided design, geoscience, and biomedical applications. The underlying problem, three-dimensional tetrahedral mesh generation, is a field of research combining various topics from discrete and computational geometry. The goal of the TetGen project is to develop and implement efficient algorithms for both research and application purposes.

Fig. 1: *Tetrahedralization of a dragon, computed with TetGen*

In 2010, the major work in TetGen was rewriting the code based on an improved tetrahedral mesh data structure. The new data structure is more efficient and memory effective compared with the original one. The performance of Delaunay tetrahedralization was improved by adding a binary space partition tree point sorting preprocess. The algorithms used in TetGen as well as their analysis are described in two recent publications [2, 3]. Two commercial licenses were sold. Based on such a license, TetGen became part of MATHEMATICA 8 by Wolfram Research.

Three-dimensional semiconductor device simulation

This is an interesting subject with respect to analysis, modeling, algorithms, numerical methods, and applications. The work focused on the following two topics: multi-dimensional vertical cavity surface emitting laser (VCSEL) simulations (project B4 in SFB 787) and silicon detector simulation for high energy and astrophysics.

In collaboration with RG 1, RG 2, the Technische Universität Berlin, and the Zuse Institute Berlin (ZIB), the research group is involved in the project B4 "Multi-dimensional modeling and simulation of VCSEL devices" within the DFG Collaborative Research Center (SFB) 787 "Semiconductor Nanophotonics: Material, Models, Devices." The joint work in this project on semi-classical device modeling resulted in a multi-species model for quantum-dot VCSELs, including a microscopic treatment of Coulomb effects [6]. Quantum dot VCSELs are lasers with optically active regions consisting of quantum dots grown on a wetting layer. The proposed multi-species model distinguishes between bulk carriers freely roaming in the whole device, carriers bound to the two-dimensional wetting layers, and carriers that are localized in the quantum dots. It describes the carrier transport

for the bulk carriers and for the carriers bound to the wetting layers by drift-diffusion equations, including scattering processes modeling the exchange between moving and localized species. In particular, the scattering rates that couple the transport equations in a nonlinear way were derived from a microscopic quantum-mechanical setting.

Silicon detector simulation for high energy and astrophysics was performed in collaboration with the European XFEL; see WIAS's Annual Research Report 2009 or http://www.xfel.eu/. This collaboration is in a final stage. It studied the evolution of dense plasma clouds in silicon detectors by simulations and experiments. Parts of the results were published in [5]. A secondary focus was on the direct support of special detector designs for very fast (up to 1 Megapixel at 5 MHz for a fraction of a second) depleted p-channel field effect transistor (DEPFET) devices for top level international experiments; compare, e.g., http://belle2.kek.jp/. The computations and algorithmic developments at WIAS contributed directly to the understanding of basic limitations. Figure 2 shows isosurfaces of the quasi-Fermi potential of a half pixel, a preliminary design by the Semiconductor Laboratory of the Max Planck Institute for Extraterrestrial Physics, Munich (http://www.hll.mpg.de/), for XFEL, where the vertical spatial resolution is 10^{-5} of the pixel height and the smallest horizontal feature is 10^{-4} of the diameter. Efficient algorithms and constructed anisotropic boundary-conforming Delaunay meshes taking a priori information into account are essential for successful simulations that are based on the Voronoi finite volume discretization. The group is collaborating with RG 1 and RG 2 on different aspects of the problem [4].

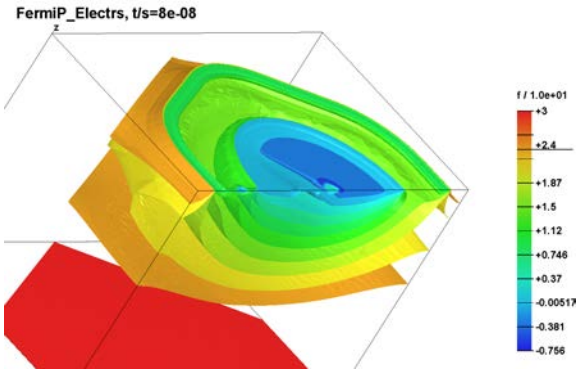


Fig. 2: *Isosurfaces of the quasi-Fermi potential of a half pixel*

Optimizing the performance of gas turbines

The block-oriented process simulator BOP combines deterministic and stochastic numerical methods to provide a framework for large-scale process simulations. This simulator includes different modes for steady state, transient, Monte Carlo, correction-curve, and homotopy simulations. The integrated BOP compiler and the modeling language MLBOP allow to generate appropriate systems of differential-algebraic equations directly from the industrial process description. BOP is licensed to Alstom Power Ltd., where it is used for simulating heavy-duty gas turbines.

The main focus of the new version BOP2.7, to be released in March 2011, lies on optimization problems. For this reason, a new deterministic optimization mode, called *MSO (Modified least-Square*

Optimization), was implemented. It complements the existing stochastic optimization mode relying on Monte Carlo-based optimization. The new mode integrates a Levenberg–Marquardt approach applied on a local trust-region model. It allows for the prediction of certain input parameters of a process while matching output parameters, e.g., measured quantities like gross power or efficiency, within certain tolerance bands. Among other things, the mode encompasses the possibility of a priori selection of the most relevant process parameters for data fitting as well as the integration of manual weighting schemes for input parameters. The main application area of the BOP MSO mode is the optimization of heat balance data for gas turbine models.

An additional extension of the BOP compiler provides a list-oriented process representation, which completely preserves the contents and the structure of the original process description file. This information enables the graphical user interface (GUI) of Alstom's "cycle-modeling framework" to provide a user-friendly editing tool for process modeling.

Besides these extensions, an additional project has been launched together with Alstom, which was originally not contractually agreed upon. This project concerns the development of a statistical analysis tool to determine the *fleet scatter* of worldwide operating gas turbines, including an experimental heat balance mode. The aim of this project consists in improving the accuracy of performance guarantees. In a first step, a script mode was implemented in BOP, which enables the execution of different analysis and correction methods for a large number of measurement data sets to prepare the needed input data for the statistical analysis.

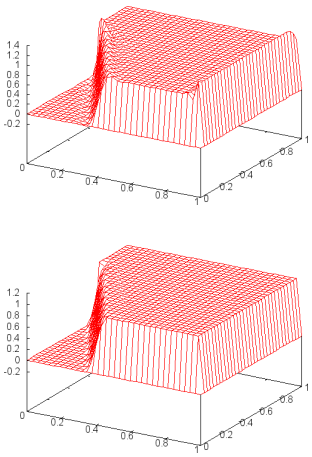


Fig. 3: *Top: SUPG solution with standard parameter containing large spurious oscillations in the layers; bottom: with parameter based on minimizing the L^2 norm of the residual and the cross wind derivative of the solution, without spurious oscillations*

Finite element methods for convection-dominated scalar equations

The efficient and accurate numerical solution of scalar convection-dominated equations is necessary in many applications, e.g., in the simulation of population balance systems as described in the Scientific Highlights article on page 43.

In collaboration with Julia Novo (Madrid), the most popular stabilized finite element approach was analyzed for time-dependent convection-diffusion equations. The main question of this approach consists in the choice of the stabilization parameter, in particular, if this parameter should depend on the length of the time step. A standard analysis works only for parameters depending on the length of the time step. However, this dependency leads to a deterioration of the method for very small time steps. With a new analysis, optimal error estimates in the appropriate norms for the discretization could be proven for stabilization parameters that are independent of the length of the time step in the case that the coefficients of the equation do not depend on time.

Another research project is the a posteriori choice of the stabilization parameters for stabilized finite element methods for stationary convection-diffusion equations. This project is joined work with Petr Knobloch (Prague). A general framework for the optimization of these parameters was developed that is based on the minimization of a functional describing the quality of the computed solution. Important components of this framework are the solution of an adjoint problem and the application of the limited memory Broyden–Fletcher–Goldfarb–Shanno (BFGS) method for solving the optimization problem. The improvements obtained for optimally chosen parameters in the streamline upwind Petrov–Galerkin (SUPG) method, with respect to a certain functional, are pre-

sented in Figure 3. The search of functionals that reflect the quality of the computed solution in an optimal way is still work in progress.

Software tools for the numerical solution of partial differential equations

Two software tools for the numerical simulation of partial differential equations are developed in the group: the simulation and visualization environment `pdelib` and the finite element code `MooNMD`. In 2010, first steps were taken to couple these codes, e.g., an interface for the exchange of meshes and solution data was implemented.

The backbone of `pdelib` is implemented in C++. In developing the code, one of the main design decisions was to store all grid and solution data in arrays. This approach allows an easy integration of numerical standard software and highly efficient core routines implemented in FORTRAN and the coupling with other packages like MATLAB and NUMPY. Another goal is portability: the code runs on all major operating systems. A major focus of the code is the Voronoi box based finite volume method. Last year brought new developments, e.g., a core module for handling higher order finite elements was implemented. Furthermore, in cooperation with RG 4, a versatile optimization tool box was developed and implemented; see also the Scientific Highlights article on page 58. The code is used for electrochemical simulations in cooperation with LG 1, for visualization in three-dimensional semiconductor device simulation, and for several projects in RG 4.

New developments in `MooNMD` include the beginning of the parallelization of the code, the extension of algorithms for solving coupled systems, like population balance systems, and first steps for simulating porous media flows. The parallelization is based on a non-overlapping domain partition, computed with METIS, and on using MPI for performing the communications. A number of data structures had to be extended. Currently, parallelized direct sparse solvers for linear systems of equations can be used. New coupling strategies and an operator-splitting approach were implemented for the simulation of population balance systems. Porous media flows are modeled with the Darcy equations. For their discretization, the Raviart–Thomas finite element was implemented, which is the first vector-valued finite element in `MooNMD`. A long-term goal consists in coupling porous media flows to incompressible flows.

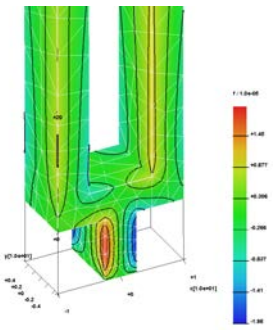


Fig. 4: *Visualization of stress in a tuning fork computed with P_2 finite elements*

References

[1] H. SI, J. FUHRMANN, K. GÄRTNER, *Boundary conforming Delaunay mesh generation*, Comput. Math. Math. Phys., **50** (2010), pp. 38–53.

[2] H. SI, K. GÄRTNER, *3D boundary recovery by constrained Delaunay tetrahedralization*, Int. J. Numer. Meth. Engng., **85** (2011), pp. 1341–1364.

[3] K. GÄRTNER, A. RAND, H. SI, N. WALKINGTON, *3D Delaunay mesh generation*, to appear in: Combinatorial Scientific Computing, U. Naumann, O. Schenk, eds., Chapman & Hall/CRC Computational Science, 2011.

[4] A. GLITZKY, K. GÄRTNER, *Existence of bounded steady state solutions to spin-polarized drift-diffusion systems*, SIAM J. Math. Anal., **41** (2010), pp. 2489–2513.

[5] J. Becker, K. Gärtner, R. Klanner, R. Richter, *Simulation and experimental study of plasma effects in planar silicon sensors*, Nucl. Inst. Meth. Phys. Research A, **624** (2010), pp. 716–727.

[6] U. Bandelow, Th. Koprucki, A. Wilms, A. Knorr, *Multi-species modeling of quantum dot lasers with microscopic treatment of Coulomb scattering*, in: Proc. 10th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD), Piscataway, USA, 2010, pp. 59–60.

[7] A. Glitzky, J. A. Griepentrog, *Discrete Sobolev–Poincaré inequalities for Voronoi finite volume approximations*, SIAM J. Numer. Anal., **48** (2010), pp. 372–391.

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 two projects in the DFG Priority Programs SPP 1180 and SPP 1204, respectively, and in the DFG Individual Grant project "Direct and inverse scattering problems for elastic waves". Thanks to the successful MATHEON evaluation in January 2010, the research group succeeded in gaining two additional projects for the whole funding period, so that it now participates in the MATHEON projects B20, C7, C11, and C30, together with colleagues from the Humboldt Universität zu Berlin, the Technische Universität Berlin, and the Zuse Institute Berlin. In addition, the short-term project D25 could be acquired. For the projects, see also pages 109 ff.

In 2010, the group further extended its successful collaboration with industry and partners from the engineering sciences. Its expertise in modeling and optimal control of phase transitions led to a funded project with the Nippon Steel Corporation, Tokyo. Moreover, the project "Modeling, simulation and optimization of multifrequency induction hardening" (MeFreSim) within the BMBF Program "Mathematics for Innovations in Industry and Services" could be acquired. Coordinated by WIAS, four scientific and two industrial partners will investigate hot topics such as control of time-dependent Maxwell's equations, model reduction, and the influence of uncertain data to further the development of a promising new heat treatment technology.

In the following, further scientific achievements of the research group in 2010 are detailed.

Optimization and optimal control

A major research topic related to the MATHEON projects C7 "Mean-risk models for electricity portfolio management and stochastic programming" and B20 "Optimization of gas transport", as well as to an industry project on gas network optimization, concerned the development of algorithmic approaches for chance-constrained optimization problems. Here, the group benefitted from an investigation of structural properties of quasi-concave distribution functions. A model for dynamic chance constraints in water reservoir management was proposed along with a numerical solution method. Other work was devoted to the investigation of deterministic and stochastic equilibrium problems with equilibrium constraints, as they arise in the ISO model of regulated electricity markets. An associated Ph.D. thesis supervised in the Research Training Group GRK 1128 "Analysis, Numerics, and Optimization of Multiphase Problems" was successfully defended and led to several publications. The latter topic raised theoretical questions such as the characterization of stability of polyhedral variational inequalities, which was investigated in [2]. Further research in nonsmooth optimization focused on error bounds and on center concepts for convex cones, both on an abstract and an applied level.

A new MATHEON project, C30 "Automatic reconfiguration of robotic welding cells", started in June 2010. Its goal is to assign the weld points situated on a workpiece to the different robots of the cell and to find the shortest collision-free path planning for each robot in a cooperation between nonlinear and discrete optimization, the latter being represented by Martin Skutella (Technische Universität Berlin). In collaboration with Matthias Gerdts (Universität der Bundeswehr, Munich), a minimum-time control problem was used to find the shortest trajectory of a robot between two weld points. In order to obtain collision-free paths, the robots and the obstacles present in the cell were represented as finite unions of convex compact polyhedra. Each object was then described by a system of linear inequalities. This description, combined with linear programming arguments, allowed to define the collision avoidance criteria and to include them as state linear constraints in the optimal control problem. The resulting formulation was finally solved with a sequential quadratic programming (SQP) method.

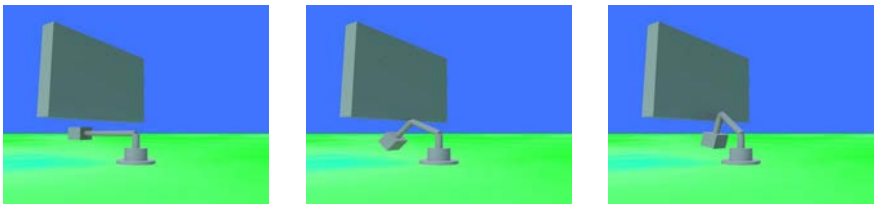


Fig. 1: *Snapshots of the collision-free motion of a robot around an obstacle*

In partial differential equation (PDE)-constrained control, the focus in 2010 was both on theoretical and numerical aspects. In a joint work with Ira Neitzel (Technische Universität Berlin) and Arnd Rösch (Universität Duisburg–Essen), a class of semilinear elliptic optimal control problems with pointwise state and control constraints was studied [4]. Assuming a sufficient second-order optimality condition and uniqueness of the dual variables, it was possible to show 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. Furthermore, second-order sufficient optimality conditions for the Moreau–Yosida regularization of semilinear state-constrained optimal control problems could be established, although the cost functional is not twice differentiable.

In collaboration with Joachim Rehberg (Research Group *Partial Differential Equations*), a control problem for the heat equation was investigated where the heat transfer coefficient in the Robin boundary conditions serves as a control variable. The problem arises, e.g., in the optimal control of the cooling section after hot-rolling of multiphase steels, as it is investigated in the SPP 1180 project (see page 111) with Wolfgang Bleck of RWTH Aachen [6]. The parabolic PDE is discussed in a new function space setting that implies higher regularity for the solution of the heat equation. This approach allows to show existence of an optimal control and the derivation of necessary and sufficient optimality conditions.

In collaboration with Timo Streckenbach (Research Group *Numerical Mathematics and Scientific Computing*), significant progress has been made in the numerical solution of control- and state-constrained optimal control problems with `pdelib`. Details can be found in the Scientific Highlights article "Optimal Control with `pdelib`" by Klaus Krumbiegel and Timo Streckenbach on page 58. As a preparation for the solution of optimal control problems related to the above-men-

tioned BMBF project *MeFreSim*, lowest-order Nedelec elements of first and second kind were implemented within `pdelib`. First simulations were carried out to solve stationary, harmonic, and time-dependent Maxwell's equations.

Inverse problems

The scattering of elastic waves by unbounded surfaces has a wide field of application, for instance, in geophysics, seismology, and nondestructive testing of materials. Compared to acoustic and electromagnetic scattering, the elasticity problems are more complicated because of the coexistence of compressional and shear waves that propagate at different speeds. Supported by the DFG Individual Grant Project "Direct and inverse scattering problems for elastic waves", significant progress could be made on the analysis of direct and inverse problems for electromagnetic and elastic diffraction gratings. Existence and uniqueness results for the first, second, third, and fourth exterior boundary value problems for the Navier equation in a three-dimensional periodic structure were established by a variational approach.

The inverse scattering of a time-harmonic elastic wave by a two-dimensional periodic structure was also investigated. The grating profile is assumed to be the graph of a piecewise linear function on which the third- or fourth-kind boundary conditions are satisfied. Extending uniqueness results for two-dimensional electromagnetic diffraction gratings [1], it was possible to determine and classify all unidentifiable grating profiles corresponding to a given incident elastic field, relying on the reflection principle for the Navier equation. Moreover, global uniqueness for the inverse problem was established with a minimal number of incident pressure or shear waves, including the resonance case where a Rayleigh frequency is allowed.

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". In [3], the stochastic model error for the measurement of line-space structures was studied. Ideally, the cross section of the bridges is of rectangular shape. The numerical reconstruction of more realistic trapezoidal shapes by both the rectangular and the trapezoidal algorithms were compared. It turned out that the height and the width measured at half of the height can be determined quite accurately by the simplified model. The results are robust with respect to typical measurement errors.

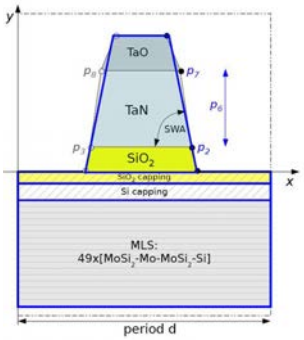


Fig. 2: *Cross section of one period of mask geometry and parameters to be reconstructed (x-coordinate of p2 and height p6)*

For the inverse algorithm in the case of biperiodic gratings, a formula for the shape derivative was developed. Though the usual $H(\mathrm{curl})$ spaces of electromagnetic fields with bounded energy are not invariant with respect to simple transformations of the geometry, the concentration on non-magnetic materials allowed for the application of classical techniques for the magnetic fields. Substituting the magnetic fields by Maxwell's equations, formulas based on electric fields were derived. The implementation is under work.

Remarkable progress has also been made for the derivation of the shape derivative for polygonal gratings. In the Ph.D. thesis of Norbert Kleemann, the theory of non-local perturbations of elliptic boundary value problems and regularity theory in weighted Sobolev spaces of Kondratiev type were used to overcome the difficulty that the shape derivative is in general not in H^1 if the interface is only piecewise smooth. The algorithmic basis for the numerical computation of the shape derivatives is a boundary-element method solver developed by Gunther Schmidt. This work was

performed within the MATHEON project D25 "Computation of shape derivatives for conical diffraction by polygonal gratings".

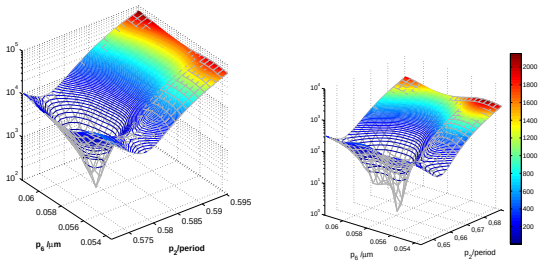


Fig. 3: *Objective functional for optimization in reconstruction procedure. Left: line-space ratio 1:2, right: line-space ratio 1:5.*

Supported by an industrial project, the above-mentioned integral equation solver for conical diffraction was extended to multi-profile gratings, especially by adding algorithms for two types of devices with an arbitrary number of material layers separated by piecewise smooth interfaces. They generalize and improve known methods for classical diffraction due to Maystre. Extending the results for one-profile gratings [5], one can show that both algorithms provide approximate solutions of conical diffraction problems if the argument of the product of the (complex) permittivities and of the (complex) permeabilities of adjacent materials is different from π .

Important progress has been made in the construction of simple high-order cubature formulas for high dimensional volume potentials and other pseudodifferential and integral operators with the concept of Approximate Approximations. Using tensor product representations of volume potentials, it is now possible to compute the values of these integrals efficiently also for very high dimensions if the density can be approximated within a given accuracy by a sum of products of univariate functions. For example, cubature formulas with convergence rate eight for harmonic potentials in R^n with $n = 200\,000$ could be obtained.

References

[1] J. ELSCHNER, G. HU, *Global uniqueness in determining polygonal periodic structures with a minimal number of incident plane waves*, Inverse Problems, **26** (2010), pp. 115002/1–115002/23.

[2] R. HENRION, B.S. MORDUKHOVICH, N.M. NAM, *Second-order analysis of polyhedral systems in finite and infinite dimensions with applications to robust stability of variational inequalities*, SIAM J. Optim., **20** (2010), pp. 2199–2227.

[3] H. GROSS, J. RICHTER, A. RATHSFELD, M. BÄR, *Investigations on a robust profile model for the reconstruction of 2D periodic absorber lines in scatterometry*, J. Eur. Opt. Soc. Rapid Publ., **5** (2010), pp. 10053/1–10053/7.

[4] K. KRUMBIEGEL, I. NEITZEL, A. RÖSCH, *Regularization error estimates for semilinear elliptic optimal control problems with pointwise state and control constraints*, WIAS Preprint no. 1480, 2010, to appear in: Comput. Optim. Appl.

[5] L. GORAY, G. SCHMIDT, *Solving conical diffraction grating problems with integral equations*, J. Opt. Soc. Amer. A, **27** (2010), pp. 585–597.

[6] P. SUWANPINIJ, N. TOGOBYTSKA, U. PRAHL, W. WEISS, D. HÖMBERG, W. BLECK, *Numerical cooling strategy design for hot rolled dual phase steel*, Steel Res. Int., **81** (2010), pp. 1001–1009.

3.5 Research Group 5 "Interacting Random Systems"

The stochastics group of WIAS continued to grow in 2010, but only slowly. In April, a new Ph.D. student started at WIAS, and in late summer two more colleagues began their work as new WIAS members. Hence, most of the year the group was rather small. Nevertheless, a number of good results was achieved, mostly in mathematical physics and stochastic interacting particle systems. The DFG Research Unit FOR 718 *Analysis and Stochastics in Complex Physical Systems*, led by the head of the research group, continued its activities, among which there were several group meetings, accompanied by a number of invited public talks. Two of the members of the research group were funded by this unit.

The main research of the group in 2010 comprised the topics described below as well as the following: description of soot formation via stochastic algorithms (see the corresponding highlight article on page 25), connectivity problems in telecommunication systems (still in its infancy), and interacting particle systems with Lennard–Jones potential.

A highlight of the year was the award of a Visiting Fellowship of the Isaac Newton Institute for Mathematical Sciences (Cambridge, UK) to Wolfgang Wagner to participate in the Program "Partial Differential Equations in Kinetic Theories". Furthermore, two internationally recognized workshops were organized by Wolfgang König at the Technische Universität Berlin for the occasions of the birthdays of Jürgen Gärtner, a former head of the group, and Erwin Bolthausen (Zurich).

Stochastic models for kinetic equations

Kinetic theory describes macroscopic features of gas flows (density, stream velocity, temperature) on the basis of the microscopic behavior of gas molecules. A common tool for the mathematical treatment of the subject are nonlinear partial integro-differential equations. These kinetic equations are closely related to stochastic interacting particle models, which are used both for analytical studies and for numerical approximations.

An interesting application of stochastic models for kinetic equations is the numerical simulation of dilute gas flows in small-scale devices (MEMS, NEMS). In collaboration with colleagues from the Massachusetts Institute of Technology (Cambridge, USA), a variance-reduced deviational particle method for the variable hard-sphere collision operator was developed in [7]. In comparison with the direct simulation Monte Carlo method, the proposed method is more suitable for simulating transport in regimes where the departure from equilibrium is small.

Fig. 1: *Schematic of the wet granulation process*

A useful property of particle models with random interactions is their robustness with respect to generalizations like the inclusion of chemical reaction mechanisms, or coagulation and fragmentation effects. In collaboration with colleagues from the Department of Chemical Engineering and Biotechnology at the University of Cambridge (UK), a stochastic particle algorithm for the solution of a five-dimensional population balance model for wet granulation was presented in [4] (see Figure 1).

Each particle consists of two types of solids (containing pores) and of external and internal liquid (located in the pores). Several transformations of particles are considered, including coalescence, compaction, and breakage.

Symmetry breaking in quasi-one-dimensional Coulomb systems

The band model of solid state physics plays a key role in understanding the electric properties of metals. In its simplest form, the model describes the metal as a periodic arrangement (crystal) of atoms and a shared cloud of (valence) electrons. The electrons are considered independent: the Coulomb repulsion between electrons is neglected. In the 1930s, Wigner suggested that, at low density, the interactions might be non-negligible and lead to a lattice structure in the electron positions, nowadays often called a *Wigner crystal*. Rigorous mathematical results on periodic structures in Coulomb systems are sparse, even for simple models. For one-dimensional systems, the existence of a Wigner crystal was rigorously proven in the 1970s in the framework of classical statistical mechanics. In dimension two, the problem is open.

In [2], the one-dimensional result is extended to a quasi-one-dimensional model of electrons moving in a long tube. With periodic or Neumann boundary conditions for the Coulomb potential, electrons arrange themselves in a periodic fashion, possibly a charge density wave instead of a Wigner crystal. The proof draws on statistical mechanics (Gibbs measures, thermodynamic limit) and probability theory (point processes, Skorokhod space), with some connections to ergodic theory and dynamical systems (cocycles). The main result says that every limit point of a suitable tight sequence of probability measures has a non-trivial behavior with respect to shifts along the tube axis.

Random media

Originally introduced in solid state physics to model amorphous materials and alloys exhibiting disorder-induced metal-insulator transitions, the Anderson model and its phenomenology have become a paradigmatic example for the relevance of effects resulting from a random background. A popular model in probability theory is the parabolic Anderson model (PAM), the discrete heat equation with random sources and sinks modeled by the Anderson Hamiltonian. A characteristic property of its solutions is the occurrence of intermittency peaks in the large time limit. They determine the thermodynamic observables extensively studied in the probabilistic literature using path integral methods and the theory of large deviations.

The rigorous study of the relation between the probabilistic approach to the PAM and the spectral theory of Anderson localization is less developed. This study is the objective of [6], where an effective random field approach is used. In particular, it offers a unified approach to the transition of the statistical moments and the integrated density of states from classical to quantum regime.

In the mathematical modeling of superfluid fermions in a random environment, random block operators play an important role. In [5], their fundamental spectral properties are studied. The results include ergodic properties, the location of the spectrum, existence and regularity of the integrated density of states, as well as Lifshitz tails. Special attention is paid to the peculiarities arising from the block structure such as the occurrence of a robust gap in the middle of the spectrum. Without randomness in the off-diagonal blocks, the density of states typically exhibits an inverse square-root singularity at the edges of the gap (left side of Figure 2). In the presence of randomness, a

Wegner estimate is established, which is valid at all energies. It implies that the singularities are smeared out by randomness, and the density of states is bounded (right side of Figure 2).

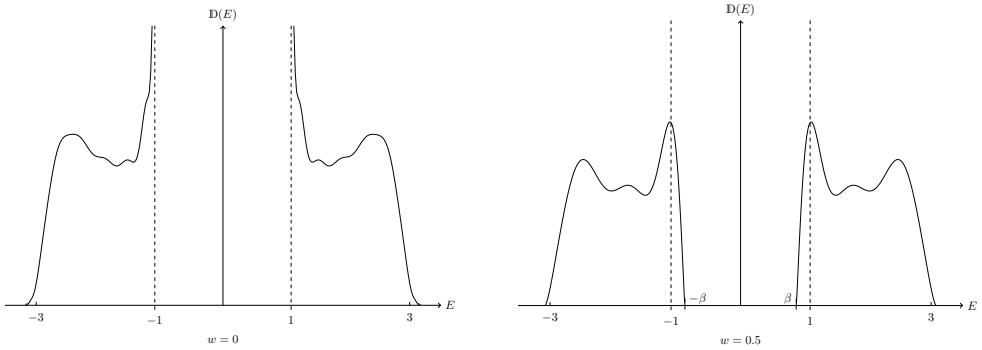


Fig. 2: *Comparison of a typical density of states in a homogeneous s-wave superconductor (left) and a disordered s-wave superconductor (right)*

Self-intersections of random walks

The description of the clumping behavior of random walks on the integer lattice is a fascinating subject since it exhibits a number of phenomena and phase transitions, depending on the dimension and the intensity of the clumping and other parameters. However, its mathematical analysis is a notoriously difficult task since the number of self-intersections is a highly discontinuous and unbounded problem. A couple of proof techniques have been derived in recent years. One contribution is the application of an explicit upper bound for the probability density of the family of local times of the walk to self-intersection local times [3]. This approach shifts the technical difficulties to the analysis of a certain variational formula with an asymptotic rescaling. Techniques of finite-element discretization are employed to describe the behavior of the rescaled quantities and to complete the description of the clumping behavior of the random walk.

Probabilistic approach to Bose–Einstein condensation

The description of an interacting Bose gas at positive temperature in the thermodynamic limit is another notoriously difficult problem. In [1], an approach using stochastic point processes and large deviations is used to obtain a representation of the limiting free energy in terms of a variational formula on the set of shift-invariant interacting point processes. This representation is valid in the non-condensing phase only, but gives new upper and lower bounds at all temperatures. This approach is not able to control the so-called *infinitely long cycles*, but describes all finitely long ones accurately.

References

[1] S. Adams, A. Collevecchio, W. König, *A variational formula for the free energy of an interacting many-particle system*, WIAS Preprint no. 1490, 2010, to appear in: Ann. Probab.

[2] M. Aizenman, S. Jansen, P. Jung, *Symmetry breaking in quasi-1D Coulomb systems*, Ann. Henri Poincaré, Theor. Math. Phys., **11** (2010), pp. 1453–1485.

[3] M. Becker, W. König, *Self-intersection local times of random walks: Exponential moments in subcritical dimensions*, WIAS Preprint no. 1532, 2010, to appear in: Probab. Theory Relat. Fields.

[4] A. Braumann, M. Kraft, W. Wagner, *Numerical study of a stochastic particle algorithm solving a multidimensional population balance model for high shear granulation*, J. Comput. Phys., **220(20)** (2010), pp. 7672–7691.

[5] W. Kirsch, B. Metzger, P. Müller, *Random block operators*, WIAS Preprint no. 1538, 2010, submitted.

[6] B. Metzger, *An effective medium approach to the asymptotics of the statistical moments of the parabolic Anderson model and Lifshitz tails*, in preparation.

[7] G. A. Radtke, N. G. Hadjiconstantinou, W. Wagner, *Low variance particle simulations of the Boltzmann transport equation for the variable hard sphere collision model*, to appear in: Rarefied Gas Dynamics, 27th International Symposium, Pacific Grove, California, July 10–15, 2010, Vol. **1333** of AIP Conference Proceedings, AIP Publishing Center, New York.

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 MATHEON projects F10 and E5 and the SFB 649 projects B5 and B7; see page 110. The group participates in two new projects won in the competitive procedure of the Leibniz Association within the *Pact for Research and Innovation* (see page 112): with the German Diabetes Center and with the Potsdam Institute for Climate Impact Research. The group also participated in the European project MASH. Moreover, members of the group were involved in several industrial contracts: with Landesbank Berlin AG on new pricing methods for Bermudan products, with HSH Nordbank on pricing and calibration of different financial instruments, and with Alstom (Switzerland) Ltd. on "Gas turbine process simulation".

Scientific highlights achieved by the research group in 2010 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 in various applications.

Highlights 2010:

- Ph.D.: Nora Serdykova, supervision: Vladimir Spokoiny
- Vladimir Spokoiny organized jointly with L. Birgé, Paris VI, and I. Johnstone, Stanford University, an Oberwolfach Workshop on "Modern Nonparametric Statistics: Going Beyond Asymptotic Minimax"
- Vladimir Spokoiny held plenary lectures at the Workshop on Mathematical Statistics, Luminy, France
- Gilles Blanchard accepted a W3-professorship offer of the University of Potsdam
- New toolbox for multiple testing
- Workshop on Validation in Statistics and Machine Learning, WIAS, October 6–7, 2010

The main fields of application are econometrics, mainly pursued within subprojects of the DFG Collaborative Research Center SFB 649, and biosciences. Within subproject F10 "Image and signal

processing in the biomedical sciences: Diffusion weighted imaging — Modeling and beyond" of the DFG Research Center MATHEON, the group focuses on applications in neuroscience.

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

The group has, in cooperation with Technische Universität Berlin, participated in the implementation of a general-purpose open multiple testing toolbox. The toolbox was written in the statistical language R and is now available on the CRAN repository. This work was supported by funding from the European network PASCAL2.

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) [5], 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.

Motivated by a growing number of application fields in the recent years, the group's research on multiple tests addresses modern challenges and open questions in this area: robust and accurate an nonasymptotic control of the type I errors (as measured by different standard criteria such as the family-wise error rate of the false discovery rate); adaptivity with respect to unknown nuisance parameters, such as the dependence structure between the test statistics, the proportion of false null hypotheses, and the alternative distribution. In particular, resampling procedures with a nonasymptotical error control were studied to this end; see [1].

One focus in statistical and machine learning at first was on novelty (or outlier) detection. This study is linked to problems belonging to both the theories of classification and of multiple testing. A second theme concerns the study of iterative and nonlinear estimation methods. A particular focus developed in 2010 was the mathematical study of partial least squares in the framework of statistical learning in a kernel space. This family of methods is known to be very efficient in practice for a large number of applications, but not yet fully understood, theoretically. Partial least squares is also intimately linked to conjugate gradient methods. The insight gained by this analysis gave rise in turn to fruitful cross-pollination and developments into the field of inverse problems (with deterministic or random noise); this direction is being actively pursued by the group; see e.g. [4]. In particular, it was established that partial least squares can be used for the regularization of statistical inverse problems by stopping with a modification of the discrepancy principle.

Within the EU-funded project MASH (Massive Sets of Heuristics, with partners in Switzerland, France, and the Czech Republic), the automated selection and combination of a very large number of hand-coded features in a collaborative environment were investigated. The focus is double, on the one hand on the development of novel, theoretically sound methods for high-dimensional heterogeneous data, and on the other hand on their application to precisely defined tasks within the project (image recognition, autonomous robotic arm).

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 makes it possible to overcome essential problems with decreased SNR in high resolution fMRI. A new unified method for adaptive smoothing and signal detection based on multiscale testing ([7]) was published. In collaboration with partners from Cornell University and the Bernstein Center for Computational Neuroscience, research on fMRI was refocused on nonlinear response models and problems in resting state fMRI. The R-package `fmri` was extended.

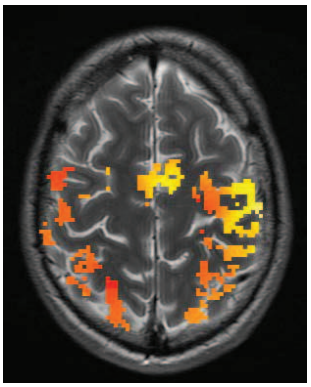


Fig. 1: *Structural adaptive segmentation: Results for a motor task*

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 investigated for their diagnostic power on clinical data by the group's partners at the University of Münster. Current research is focused on models for high angular resolution DWI (HARDI), in particular on tensor mixture models. Such models are suitable to describe subvoxel effects like fiber crossings that can not be addressed by DTI.

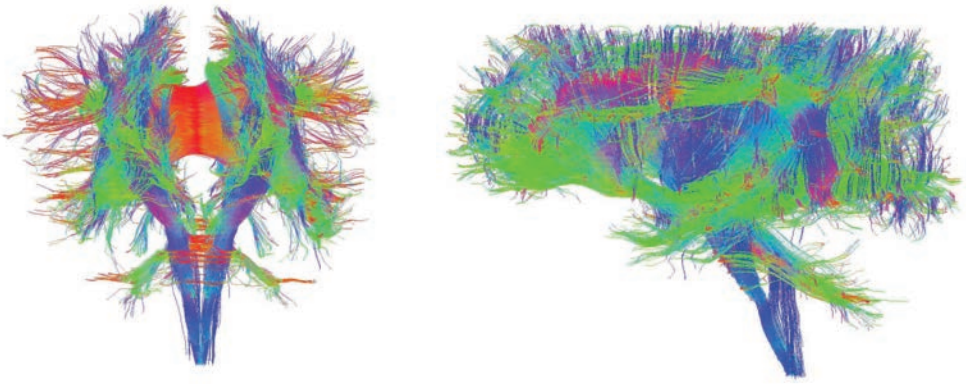


Fig. 2: *Fiber tracks exceeding at least 100 voxels obtained using tensor mixture models with maximum order 5. Color codes the local fiber direction.*

A new approach for smoothing HARDI data is under development. The R-package `dti` was extended to include models for HARDI data and streamline fiber tracking.

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. In particular, there is an increasing demand for effective solutions to optimal control problems for real-world high-dimensional problems.

Highlights 2010:

- Professorships: Denis Belomestny got a W3 offer of the University of Duisburg-Essen and a W2 offer of the University of Twente
- Prolongation of the industrial contract with HSH Nordbank
- Prolongation of MATHEON E5 project "Statistical and numerical methods in modeling of financial derivatives and valuation of risk"
- Monograph: PETER FRIZ, *Multidimensional Stochastic Processes as Rough Paths. Theory and Applications* Cambridge Studies in Advanced Mathematics, 670 p., Cambridge University Press, 2010
- Peter Friz gained an ERC Starting Grant
- Peter Friz acted as organizer of several meetings on rough path, e.g., as part of the 5th European Congress of Mathematics (5ECM), the 33rd Conference on Stochastic Processes and Their Applications (SPA09), and within the 2010 Program on Stochastic Partial Differential Equations at the Newton Institute in Cambridge

In the area of pricing and hedging high-dimensional American (Bermudan) options, the regression-based methods studied in [2] and [3] were extended and suited for application to real-life optimization problems, such as portfolio liquidation, optimization under transaction costs, etc.

In the context of dual pricing of American options, a new stability result was obtained concerning the construction of surely optimal dual martingales. Due to this result, a new regression-based dual evaluation algorithm for computing upper bounds to American option prices is developed, which, in contrast to the usual algorithms known so far, does not require a certain given "input" approximation to the corresponding optimal stopping problem (Snell envelope). Moreover, the new algorithm also produces lower approximations to the option value at the same time.

In electricity markets, the evaluation of (swing) options requires efficient algorithms for multiple stopping problems. In this context, a breakthrough was achieved, where a new dual representation for multiple stopping problems was developed. This representation was extended to much more general payoff profiles. In the extended setting, it is possible to treat more realistic energy (swing) options that may include volume constraints and refraction periods.

Many problems in risk management require optimization methods for advanced risk measures and utility functionals rather than an optimization of the ordinary expectation and a minimization of the standard Value at Risk. The newly developed representation methods in [6], which allow for a numerical treatment of such problems, were studied further for a particular class of robust functionals, the so-called *g-expectations*. The development of efficient numerical algorithms for optimization with respect to these functionals was started.

Recently, there is a growing trend to embed funds switching rights into minimum return guarantee products. The payoff of these products is given by the maximum of the account value and a guaranteed value, where the switching right is of American type. This approach implies an optimal stopping problem where the risk management of such products relies on the most risky strategy. It

is shown that, within the class of jump-diffusions, the optimal strategy is deterministic if and only if the jump part of the underlying account vanishes.

Another research theme in the project is the application of rough path analysis to finance. Rough path analysis allows for a fresh view on Ito's theory of stochastic differential equations. There are various connections to quantitative and numerical finance, for instance via cubature-based (quasi-) Monte Carlo methods, variance options, and analytic properties of stochastic volatility models.

References

[1] S. Arlot, G. Blanchard, E. Roquain, *Some non-asymptotic results on resampling in high dimension, I: Confidence regions* and *II: Multiple tests*,Annals of Statistics, **38** (2010), pp. 51–82 and 83–99.

[2] D. Belomestny, *On the rates of convergence of simulation-based optimization algorithms for optimal stopping problems,* Ann. Appl. Probab., **21(1)** (2011), pp. 215–239.

[3] D. Belomestny, A. Kolodko , J. Schoenmakers, *Regression methods for stochastic control problems and their convergence analysis*, SIAM J. Control Optim., **48(5)** (2010), pp. 3562–3588.

[4] G. Blanchard, P. Mathé, *Conjugate gradient regularization under general smoothness and noise assumptions*, J. Inverse Ill-Posed Probl., **18** (2010), pp. 701–726.

[5] E. Diederichs, A. Juditski, V. Spokoiny, Chr. Schütte, *Sparse non-Gaussian component analysis*, IEEE Trans. Inform. Theory, **56** (2010), pp. 3033–3047.

[6] V. Krätschmer, J. Schoenmakers, *Representations for optimal stopping under dynamic monetary utility functionals,* SIAM J. Financial Math., **1** (2010), pp. 811–832.

[7] J. Polzehl, H.U. Voss, K. Tabelow, *Structural adaptive segmentation for statistical parametric mapping*, NeuroImage, **52** (2010), pp. 515–523.

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. In 2010 Pierre-Étienne Druet obtained the Nachwuchspreis (Young Scientists' Prize) of the Leibniz Association for the best dissertation in the fields of natural and technical sciences. His thesis "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" represents a mathematical breakthrough because the awardee proved existence and uniqueness for the fully coupled system. The extremely difficult problem arises out of a materials science application in the context of an ongoing interdisciplinary project on the production of solar silicon. The award is endowed with 3,000 Euros.

Fig. 1: *Pierre-Étienne Druet (left) obtained the Young Scientists' Prize of the Leibniz Association*

2. In 2010, the years of successful collaboration between Pierluigi Colli (Pavia), Pavel Krejčí (Prague), Elisabetta Rocca (Milano), and Jürgen Sprekels (WIAS) devoted to the study of nonlocal temperature-dependent models of multi-phase transition systems culminated in a satisfactory

conclusion. In [1], for the first time the case could be handled that both specific heat and heat conductivity of the material exhibit a physically meaningful dependence on both the absolute temperature θ and the order parameter vector χ. Also, the assumptions on the free energy of the system were very general and included the case that the convex component of the free energy may be singular.

The main mathematical obstacle that had to be overcome in the proof was the fact that the governing field equations couple a vectorial integro-differential inclusion for χ in a highly nonlinear way with a quasilinear internal energy balance ruling the evolution of the absolute temperature. With a delicate interplay between cut-off techniques, approximation methods, maximum principle arguments, and Moser iteration techniques, general existence and uniqueness results could be established.

3. In collaboration with partners from the National Institute of Chemistry in Slovenia, members of the research group achieved a significant breakthrough in the modeling of many-particle electrodes used in rechargeable lithium-ion batteries. The electrode consists of many nano-sized particles that serve to reversibly store and release lithium atoms during the process of charging and discharging. Until 2010, the literature on the storage problem was based on the assumption that the storage particles are concurrently loaded with lithium so that their lithium content is the same at any instant of time. That model was disproved by the project partners, and they proposed a new model where the loading process is a sequential one according to the rule *one particle after the other*.

The chemical essentials of the new many-particle model are described in the paper "The thermodynamic origin of hysteresis in insertion batteries" [3], the corresponding mathematical model and numerical simulations are treated in the article "Hysteresis and phase transition in many-particle storage systems" [4], and the mathematical analysis is found in the preprint "Blow-up versus boundedness in a non-local and non-linear Fokker–Planck equation" [5].

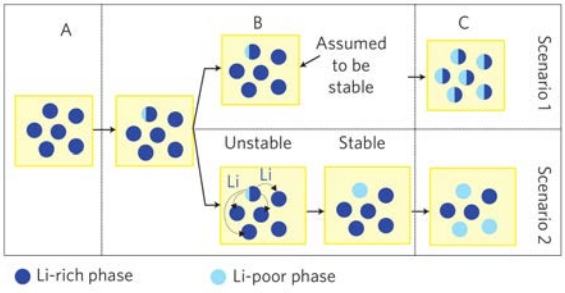


Fig. 2: *Two possible scenarios for the behavior of many-particle electrodes during charging*

4. The group contributed with four projects to the successful evaluation of the DFG Research Center MATHEON that was granted a third funding period until 2014:

C9: "Simulation and optimization of semiconductor crystal growth from the melt controlled by traveling magnetic fields"

C10: "Modelling, asymptotic analysis and numerical simulation of the dynamics of thin film nanostructures on crystal surfaces"

C17: "Adaptive multigrid methods for local and nonlocal phase-field models of solder alloys"

C26: "Storage of hydrogen in hydrides"

Funded projects with industrial collaboration

In the past years, the research group has acquired large competence in mathematical modeling, analysis, and simulation of technical processes in the context of production of new materials. The following two 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. Originally, the project should have ended in December 2010. However, due to its success in November 2010 to produce large silicon crystals of rectangular shape, the project will be continued until June 2011.

During the last year, the WIAS team, guided by Wolfgang Dreyer, Olaf Klein, and Jürgen Sprekels, contributed with simulations of the global temperature field inside the growth device and of the transport of unwanted substances in the melt in front of the liquid-crystal interface. Furthermore, a new and necessary study concerning the chemical composition of the crucible coating was started.

Among the technological objectives is the favorable influence of applied time-dependent magnetic fields on the flow pattern in the melt. In particular, the distribution of unwanted substances in the melt is of major interest. The Figure shows a three-dimensional simulation of the coupled system of Navier–Stokes and diffusion equations. For a rectangular melt geometry, a snapshot is given exhibiting the distribution of oxygen without and with two variants of an applied magnetic field.

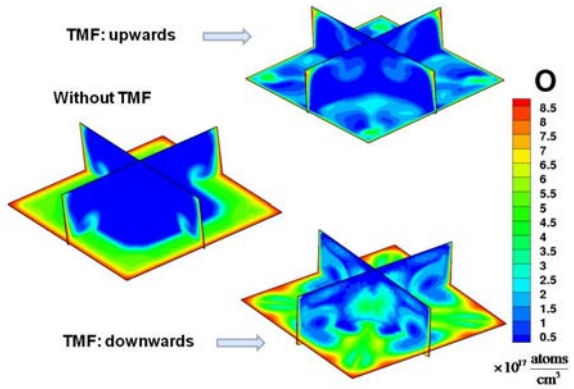


Fig. 3: *Influence of a traveling magnetic fields on the distribution of unwanted oxygen in a 3D melt flow*

2. Barbara Wagner from this group and Andreas Münch from the University of Oxford successfully completed an industrially funded project to design a software package for a multi-wall device for surface coating, financed until April 2010. Two new important achievements can be announced.

A new tool to treat stability analysis was added to the existing software package including flow simulation with a free liquid–air interface, elastomer simulation with a solid–liquid interface, and

coupling of both phenomena. It offers the possibilities of applying the stability analysis either to the weak or to the strong version of the underlying PDE system. Interestingly, both variants do not lead to the same stability results. A study of their equivalence currently remains an open problem. However, for both variants numerical codes were already developed and tested. From the experimental point of view, the stability analysis of the strong PDE system gives better results.

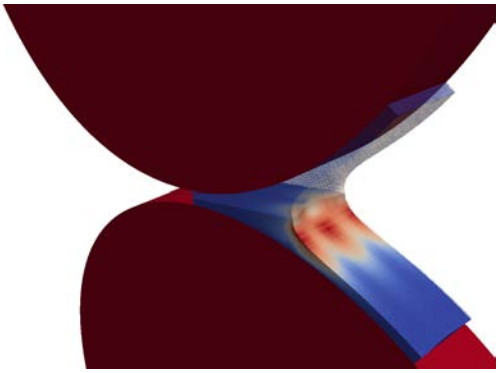


Fig. 4: *Disturbed liquid flow between two stiff rolls*

In the context of the industrial project, a new model was established and used for simulations. The model aims to describe the sedimentation of discrete particles in a flow field. The challenge here is the formulation of electrochemical and hydrodynamical interaction. This part of the project is carried out in collaboration with partners from the University of California, Los Angeles.

Funded under Priority Programs of the German Research Foundation

Dirk Peschka and Barbara Wagner participated in the DFG Priority Program SPP 1506 "Transport Processes at Fluidic Interfaces" with the funded project "Dynamics of viscous multi-layer systems with free boundaries". Related to that project is the paper "Interface morphologies in liquid/liquid dewetting" [2].

Selected MATHEON projects

1. In the project C10 "Modelling, asymptotic analysis and numerical simulation of the dynamics of thin film nanostructures on crystal surfaces" , Maciek Korzec, Pete Evans, and Barbara Wagner, jointly with Andreas Münch, University of Oxford, continued the study of self-assembly of quantum dots on crystalline substrates. The mathematical model by Korzec and Evans, described in [6], was extended by a stochastic disturbed atomic flux. New numerical simulations of the extended model show that higher deposition rates lead to an increased island density of smaller quantum dots. The corresponding results are documented in the thesis [7].

2. One of the various models that are developed in the project C26 "Storage of hydrogen in hydrides" by Wolfgang Dreyer, Clemens Guhlke, and Robert Huth. jointly with Michael Herrmann, University of Oxford, consists of an initial and boundary value problem for the nonlocal and nonlinear Fokker–Planck equation. In an interdisciplinary study between the C26 group, Joachim Rehberg

and Alexander Mielke from the Research Group *Partial Differential Equations*, and in collaboration with Michael Winkler from the University Duisburg-Essen, three important problems could be solved: 1. Existence and uniqueness for small times; 2. Existence and uniqueness for large times if the load function remains within the interval $(0, 1)$; 3. The positivity of the solution, which represents a probability density. The various proofs, given in [5], rely on semi-group theory and on the modern theory of interpolation spaces.

Ph.D. students

Wolfgang Dreyer, Jürgen Sprekels, and Barbara Wagner, jointly with other partners, guide and supervise nine Ph.D. students, within the DFG Research Center MATHEON, in collaboration with the Technische Universität Berlin and the Humboldt-Universität zu Berlin, and in further third-party funded projects.

In 2010, Maciek Korzec successfully defended his dissertation on "Continuum modelling, analysis and simulation of the self-assembly of thin crystalline films" with *summa cum laude* at the Technische Universität Berlin. The mathematical core of his thesis concerns the analysis of the quasilinear PDE of sixth order

$$u_t - \frac{\delta}{2}(u^2)_x = (u_{xx} + u - u^3_{xxxx}) \quad \text{with} \quad u(x,0) = u_0(x)\,. \tag{1}$$

In particular, he was able to show the global existence of unique weak solutions to (1) in the case of periodic boundary conditions. The function u gives the slope of facets of a growing crystal surface. The PDE arises within the setting of a dimensionally reduced model.

The various Ph.D. projects in the research group are based on continuum models of large complexity. They comprise various couplings of different phenomena. Examples are (i) diffusion and mechanical stresses, (ii) liquid flow in magnetic fields with heat conduction, (iii) complex thin film/substrate interactions. Thus, there arise involved initial-boundary value problems for nonlinear coupled systems of partial differential equations.

Miscellaneous

Jürgen Sprekels translated the book by Fredi Tröltzsch (Technische Universität Berlin) "Optimal Control of Partial Differential Equations: Theory, Methods and Applications" into English. It appeared as Vol. 112 in the AMS series Graduate Studies in Mathematics.

Barbara Wagner received a call to a professorship in Mathematical Models of Photovoltaics at the Technische Universität Berlin.

References

[1] P. COLLI, P. KREJČÍ, E. ROCCA, J. SPREKELS, *A nonlocal quasilinear multi-phase system with nonconstant specific heat and heat conductivity*, J. Differential Equations, **251** (2011), pp. 1354–1387.

[2] K. Kostourou, D. Peschka, A. Münch, B. Wagner, S. Herminghaus, R. Seemann, Interface morphologies in liquid/liquid dewetting, to appear in: Chem. Eng. Proc.

[3] W. Dreyer, J. Jamnik, C. Guhlke, R. Huth, J. Moškon, M. Gaberšček, *The thermodynamic origin of hysteresis in insertion batteries*, Nature Materials, **9** (2010), pp. 448–453.

[4] W. Dreyer, C. Guhlke, M. Herrmann, *Hysteresis and phase transition in many-particle storage systems*, Contin. Mech. Thermodyn., **23(3)** (2011), pp. 211–231.

[5] W. Dreyer, R. Huth, A. Mielke, J. Rehberg, M. Winkler, *Blow-up versus boundedness in a nonlocal and nonlinear Fokker–Planck equation*, WIAS Preprint no. 1604, 2011.

[6] M.D. Korzec, P.L. Evans, *From bell shapes to pyramids: A continuum model for self-assembled quantum dot growth*, Physica D, **239(8)** (2010), pp. 465–474.

[7] M.D. Korzec, *Continuum modelling, analysis and simulation of the self-assembly of thin crystalline films*, Ph.D. Thesis, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, 2010.

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

The Leibniz group, which closely cooperates with the Research Group *Numerical Mathematics and Scientific Computing* (RG 3), was established in the framework of the competition procedure of the Leibniz Association, as a part of a research network joining WIAS, the Freie Universität Berlin, the Potsdam Institute for Climate Impact Research, and the University of Erlangen. Based on funding for the years 2008–2010, the network focused on coupled flow processes in electrochemical systems and on the coupling between flow processes in the atmosphere and the soil. The Scientific Highlights article on page 35 summarizes the results of the network obtained during the period of its existence. Following the suggestion of the commission that evaluated WIAS in 2010 (see Foreword), the investigations performed by the Leibniz group will be continued in the framework of RG 3.

Recent investigations focused on deepening the understanding of various options to discretize the Navier–Stokes equation with schemes allowing for strong mass conservation at the discrete level. In this respect, the Scott–Vogelius finite element guarantees pointwise mass conservation. Continuing its investigation, the interconnection of the element with stabilization methods for the Taylor–Hood element was studied [3]. Furthermore, a convergence proof for a discretization scheme that couples the Scott–Vogelius finite element for fluid flow to the Voronoi box based finite volume method for the transport of a dissolved species was given [4]. First steps towards a finite volume scheme for the Navier–Stokes equations with exact mass conservation were taken. Based on discrete vector calculus, finite volume schemes for the Stokes equations were investigated which, in analogy to the continuous case, are equivalent to a fourth-order equation for a discrete stream function [2].

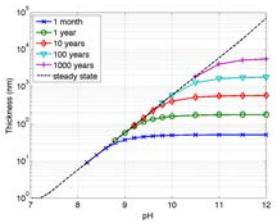


Fig. 1: *Evolution of thickness of the corrosion layer for different pH values of the surrounding fluid [5]*

The main application area of the group was electrochemistry. One focus of the work was on heterogeneous electrocatalyis. The desorption and re-adsorption of reactive intermediates at catalytic surfaces was investigated using numerical and asymptotic modeling. It was found that, on a qualitative level, macroscopic equations allow to explain the experimentally established effect that increased catalyst loading leads to a decrease of the fraction of intermediates in the reaction products [1].

The evolution of the oxide layer during corrosion of carbon steel under anoxic conditions can be described by a free boundary value problem for a Nernst–Planck–Poisson system describing the transport of electrons, iron ions and oxygen vacancies. A one-dimensional finite volume model for this so-called *Diffusion Poisson Coupled Model (DPCM)* implemented mainly at the French Alternative Energies and Atomic Energy Commission CEA was considerably improved using numerical techniques established in the group [5], see also Figure 1.

References

[1] J. Fuhrmann, H. Zhao, H. Langmach, Y. Seidel, Z. Jusys, R.-J. Behm, *The role of reactive reaction intermediates in two-step heterogeneous electro-catalytic reactions: A model*

study, WIAS Preprint no. 1522, 2010, to appear in: Fuel Cells (available online, DOI: 10.1002/fuce.201000112).

[2] R. Eymard, Th. Gallouët, R. Herbin, A. Linke, *Convergence of a finite volume scheme for the biharmonic problem*, WIAS Preprint no. 1482, 2010, submitted.

[3] A. Bowers, B. Cousins, A. Linke, L. Rebholz, *New connections between finite element formulations of the Navier–Stokes equations*, J. Comput. Phys., **229** (2010), pp. 9020–9025.

[4] J. Fuhrmann, H. Langmach, A. Linke, *A numerical method for mass conservative coupling between fluid flow and solute transport*, Appl. Numer. Math., **61** (2011), pp. 530–553.

[5] Ch. Batallion, F. Bouchon, C. Chainais-Hillairet, J. Fuhrmann, E. Hoarau, R. Touzani, *Numerical methods for the simulation of a corrosion model in a nuclear waste deep repository*, WIAS Preprint no. 1575, 2010, submitted.

3.9 Leibniz Group 2 *"Modeling of Damage Processes"*

Within the competitive procedure of the Leibniz Association in the Pact for Research and Innovation, Dorothee Knees and Christiane Kraus successfully applied for a grant that provides the basis for the Leibniz Group 2. The group was formed at WIAS in 2009, working on the modeling, analysis, and simulation of damage processes.

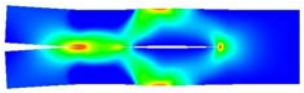


Fig. 1: *Stress distribution in a cracked body with self-contact (D. Knees (LG 2), A. Schröder (HU Berlin))*

Materials enabling the functionality of technical devices change their microstructure over time. For instance, phase separation and damage processes take place. The group works on the analytical and numerical modeling of *phase separation* and *damage processes* in alloys with the intention to predict and optimize the strength and lifetime of solder joints. To this end, the existing framework of Cahn–Hilliard systems is extended by coupling these systems with a unidirectional inclusion for an internal variable, describing damage processes. For these systems, appropriate notions of weak solutions and existence results are established, based on regularization methods and higher integrability properties for the strain tensor. For numerical investigations on this topic, the reader is referred to the Scientific Highlights article by Rüdiger Müller on page 53.

As a further topic, the link between rate-dependent (viscous) damage and fracture models and their rate-independent counterparts was investigated. In cooperation with A. Schröder (Humboldt University of Berlin), convergence results for the simulation of crack propagation were obtained and verified by numerical studies. In particular, relations between the discretization parameters were identified guaranteeing the convergence of the fully discretized, viscous models to the vanishing viscosity model. The proofs rely on regularity properties of the displacements and the damage variables. Within the short-term MATHEON project C35 and in cooperation with colleagues from the Institute of Applied Mathematics and Information Technology IMATI, Pavia, uniform regularity estimates were derived for minimizers of a large class of functionals.

The research group participates in the DFG Research Center MATHEON with the projects C32 "Modeling of phase separation and damage processes in solder alloys" and C35 "Global higher integrability of minimizers of variational problems with mixed boundary conditions".

Christiane Kraus participates in the interdisciplinary Research Unit 563 *Micro-Macro Modeling and Simulation of Liquid–Vapor Flows* of DFG and CNRS with the project "Modeling and sharp interface limits of generalized Navier–Stokes–Korteweg systems".

Fig. 2: *Participants of the 6th Singular Days*

The International Workshop "6th Singular Days on Asymptotic Methods for PDEs", organized by Dorothee Knees (LG 2) and Annegret Glitzky (RG 1), took place at WIAS from April 29 through May

1, 2010. The lectures focused on regularity results for elliptic and parabolic PDEs on nonsmooth domains and with nonsmooth coefficients, on numerical methods and on applications in physics and mechanics. Partial financial support by the DFG is gratefully acknowledged.

A Facts and Figures

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

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

A.1.1 Calls

1. D. Belomestny, W2 professorship, October 12, University of Twente, Faculty of Electrical Engineering, Mathematics and Computer Science (associate professorship).
2. ———, W3 professorship, August 30, Universität Duisburg-Essen, Fakultät für Mathematik.
3. K. Krumbiegel, Junior professorship, May 20, Universität Leipzig, Fakultät für Mathematik und Informatik.
4. B. Wagner, W2 professorship, August 9, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften.

A.1.2 Awards and Distinctions

1. P.-É. Druet, *Young Scientists' Prize 2010 of the Leibniz Association*, November 24.
2. D. Knees, *Robert Bosch Stiftung: Fast Track Scholarship*, 2008–2010.
3. K. Krumbiegel, *Award for best Ph.D. thesis, Dies Academicus 2010, Universität Duisburg-Essen*, June 23.
4. A. Mielke, *Coordinator of the Theoretical Mechanics Group of the Centro di Ricerca Matematica "Ennio De Giorgi", Pisa, Italy*.
5. ———, *Member of the Executive Committee of the International Society for Interaction of Mathematics and Mechanics (ISIMM)*.
6. J. Sprekels, *Coordinator of the International Mathematical Science Institutes (IMSI)*.

A.1.3 Ph.D. Theses

1. L. Panizzi, *On a mathematical model for case hardening of steel*, Scuola Normale Superiore di Pisa, Classe di Scienze, supervisor: Prof. Dr. D. Hömberg, March 5.
2. M. Roland, *Numerische Simulation von Fällungsprozessen mittels Populationsbilanzen*, Universität des Saarlandes, Naturwissenschaftlich-Technische Fakultät I, supervisor: Prof. Dr. V. John, May 19.
3. S. Schmidt, *Das parabolische Anderson-Modell mit Be- und Entschleunigung*, Universität Leipzig, Fakultät für Mathematik und Informatik, supervisor: Prof. Dr. W. König, December 15.
4. Th. Surowiec, *Explicit stationarity conditions and solution characterization for equilibrium problems with equilibrium constraints*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisors: Priv.-Doz. Dr. R. Henrion, Prof. Dr. J. Outrata, January 27.
5. M. Korzec, *Continuum modeling, analysis and simulation of the self-assembly of thin crystalline films*, Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Priv.-Doz. Dr. B. Wagner, October 11.
6. N. Serdyukova, *Adaptive estimation in regression and complexity of approximation of random fields*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. V. Spokoiny, May 14.

7. M. Thomas, *Rate-independent damage processes in nonlinearly elastic materials*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. A. Mielke, February 16.

A.1.4 Undergraduate-degree Supervision

1. A. Bumb, *Energiefreisetzungsrate in Piezomaterialien* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. A. Mielke, February 3.
2. D. Erhard, *Weakly self-avoiding walk in a trap* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, September 20.
3. J. Hähnel, *Exakte Lifshitz-Tails für den Anderson-Operator mit Weibull-verteiltem Potential* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, May 4.
4. S. Käbisch, *Anwendung eines halbglatten Newtonverfahrens zur Auswertung von Dilatometerdaten* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, December 2.
5. A. Kamprad, *Bewertung aggregierter Risiken* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Priv.-Doz. Dr. V. Krätschmer, November 24.
6. S. Reichelt, *Homogenisierung eines Modells zum Risswachstum* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. A. Mielke, August 12.
7. Ch. Ryll, *Deterministische und evolutionäre Strategien zur Approximation von Pareto-Fronten in der multikriteriellen nichtlinearen Optimierung* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, December 2.
8. M. Saadi, *Analytische/Numerische Modellierung mobiler Nutzer durch Markov'sche Ankunftsprozesse* (diploma thesis), Universität Leipzig, Fakultät für Mathematik und Informatik, supervisor: Prof. Dr. W. König, May 27.
9. S. Schwabecher, *Prämienaufteilung mit Risikomaßen als Prämienprinzipien* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Priv.-Doz. Dr. V. Krätschmer, April 29.
10. St. Sickora, *Risikolose Absicherung fondsgebundener Lebensversicherungen* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Priv.-Doz. Dr. V. Krätschmer, August 16.
11. K. Steinberg, *The parabolic Anderson models with catalysts in different state spaces* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 11.
12. A. Stephan, *Dynamisches stochastisches Modell zur integrierten Betrachtung von Markt- und Kreditrisiko* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Priv.-Doz. Dr. V. Krätschmer, May 13.
13. S. Suske, *Risikominimierende Absicherung fondsgebundener Lebensversicherungen* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Priv.-Doz. Dr. V. Krätschmer, July 27.
14. H. Tessemo, *Portfoliooptimierung in Hidden Markov Modellen* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Priv.-Doz. Dr. V. Krätschmer, January 8.

15. T. Wolff, *The parabolic Anderson model from the perspective of a moving point potential* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 11.

16. St. Zunhammer, *Rissausbreitung in elastoplastischen Materialien* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. A. Mielke, June 22.

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)

"Verbundprojekt MeFreSim: Modellierung, Simulation und Optimierung des Mehrfrequenzverfahrens für die induktive Wärmebehandlung als Bestandteil der modernen Fertigung" (Joint project MeFreSim: Modeling, simulation and optimization of multifrequency induction hardening as part of modern manufacturing technology); project coordination and subproject "Gesamtmodell, Analysis, Gesamtsimulator" (Modeling, analysis, process simulator; in RG 4)

– **Optische Technologien** (Optical technologies)

"INLAS: Integriert-optische Komponenten für Hochleistungs-Laserstrahlquellen" (Integrated-optical components for high power laser beam sources), together with Ferdinand-Braun-Institut für Höchstfrequenztechnik Berlin; subproject "Erforschung und Entwicklung von innovativen hybrid-integrierten Diodenlaser-Komponenten und Systemen" (Research and development of innovative hybrid integrated laser diode components and systems; in RG 2)

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 (DFG, 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" (until 5/10, 1 position at WIAS; in RG 6)

B20: "Optimization of gas transport" (1.5 positions at ZIB, 1 position at HU Berlin, 0.5 position at WIAS; in RG 4)

C7: "Mean-risk optimization of electricity production in liberalized markets" (1 position at HU Berlin; in RG 4)

C9: "Numerical simulation and control of sublimation growth of semiconductor bulk single crystals", new title since June 2010: "Simulation and optimization of semiconductor crystal growth from the melt controlled by traveling magnetic fields" (1 position at WIAS, 1 position at TU Berlin; in RG 7)

C10: "Modelling, asymptotic analysis and numerical simulation of the dynamics of thin film nanostructures on crystal surfaces" (1,5 positions at WIAS; in RG 7)

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

C11: “Modeling and optimization of phase transitions in steel” (1 position at WIAS; in RG 4)

C14: “Macroscopic models for precipitation in crystalline solids” (until 5/10, 1 position at WIAS, 1 position at TU Berlin; in RG 7)

C17: “Adaptive multigrid methods for local and nonlocal phase-field models of solder alloys” (1 position at FU Berlin; in RG 7)

C18: “Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys” (1 position at WIAS; in RG 1)

C26: “Storage of hydrogen in hydrides” (0.5 position at WIAS; in RG 7)

C30: “Automatic reconfiguration of robotic welding cells” (0.5 position at WIAS, 0.5 position at TU Berlin; in RG 4)

C32: “Modeling of phase separation and damage processes in alloys” (from 6/10, 0.5 position at WIAS; in LG 2)

C35: “Global higher integrability of minimizers of variational problems with mixed boundary conditions” (7/10–12/10, 0.75 position at WIAS; in LG 2)

D4: “Quantum mechanical and macroscopic models for optoelectronic devices” (until 5/10, 1 position at WIAS; in RG 1)

D8: “Nonlinear dynamical effects in integrated optoelectronic structures” (0.5 position at WIAS, 0.5 position at HU Berlin; in RG 2)

D14: “Nonlocal and nonlinear effects in fiber optics” (1 position at WIAS; in RG 1 and RG 2)

D22: “Modeling of electronic properties of interfaces in solar cells” (from 8/10, 1 position at WIAS; in RG 1)

D25: “Computation of shape derivatives for conical diffraction by polygonal gratings” (7/10–12/10, 0.75 position at WIAS; in RG 4)

E1: “Microscopic modelling of complex financial assets” (until 5/10, 1 position at WIAS; in RG 5)

E5: “Statistical and numerical methods in modelling of financial derivatives and valuation of risk” (until 5/10 2 positions at WIAS, since 6/10 1,5 positions at WIAS; in RG 6)

F10: “Image and signal processing in the biomedical sciences: Diffusion weighted imaging — Modeling and beyond” (from 6/10, 1 position at WIAS; in RG 6)

Z1.4: “Innovations in mathematics education for the engineering science” (until 5/10, 1 position at TU Berlin; 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, optimization 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)

– **Priority Program SPP 1506: "Fluide Grenzflächen" (Transport Processes at Fluidic Interfaces)**

"Mathematical modeling, analysis, numerical simulation of thin liquid bilayers and validation experiments" (in RG 7)

– **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)**

"Adaptive Parameterbestimmung in stabilisierten Finite-Element-Methoden für konvektionsdominante Gleichungen" (Adaptive parameter estimation in stabilized finite element methods for convection-dominated equations: in RG 3)

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

"Erzeugung von Vakuumultraviolett- und Terahertz-Pulsen durch plasmagenerierende Femtosekunden-Laserpulse im Freiraum und in geführten Geometrien" (Vacuum ultraviolet and terahertz pulse generation in bulk media and guided geometries based on plasma generating femtosecond light pulses; in RG 2)

"Modellierung und scharfe Grenzwerte von lokalen und nicht-lokalen verallgemeinerten Navier-Stokes-Korteweg-Systemen" (Modeling and sharp interface limits of local and non-local generalized Navier–Stokes–Korteweg systems, in the framework of the DFG-CNRS Research Unit 563 "Micro–Macro Modelling and Simulation of Liquid–Vapor Flows"; in RG 7 and LG 2)

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

– Bilateral cooperation with the National Academy of Sciences of Ukraine: "Kollektive Phänomene und Multistabilität in Netzwerken von dynamischen Systemen" (Collective phenomena and multistability in networks of dynamical systems; in RG 2)

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

Leibniz-Gemeinschaft (Leibniz Association), Bonn and Berlin

– **Wettbewerbliches Verfahren im "Pakt für Forschung und Innovation" (Competitive Procedure in "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)

"ECONS: Evolving Complex Networks – Regionales Ressourcen-Management unter den Bedingungen des Umwelt- und demografischem Wandels" (Regional ressource management under environmental and demographic change), joint project of Potsdam Institute for Climate Impact Research, Leibniz Institute of Freshwater Ecology and Inland Fisheries, German Institute of Economic Research, and WIAS (in RG 6)

"Multiplizität, Modellvalidierung und Reproduzierbarkeit in hochdimensionalen Microarray-Daten" (Multiplicity, model validation, and reproducibility in high-dimensional microarray data), joint project of German Diabetes Center in Duesseldorf, University of Duesseldorf, and WIAS (in RG 6)

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

– 2 scholarship holders (in RG 3 and RG 5) see page 164

Deutscher Akademischer Austauschdienst (DAAD, German Academic Exchange Service), Bonn

– PROCOPE: "Adaptive multiple Testverfahren mit hohen Dimensionen" (Adaptive multiple testing procedures in high dimensions; in RG 6)

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

Technologiestiftung Berlin (Technology Foundation Berlin)

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

International Projects

- ERC Starting Independent Researcher Grant “Rough path theory, differential equations and stochastic analysis” (P. Friz in RG 6)
- EU Collaborative Project “MASH — Massive Sets of Heuristics” (in RG 6)
- Researchers of RG 6 participated in the EU Network of Excellence PASCAL2.

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)
- Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin: “2D- und 3D-Simulationen zu bestimmten Modellen von Dünnschichtsolarzellen auf der Basis von $CuInS_2$-Chalkopyrit” (2D and 3D simulations of the particular thin-film solar-cell models based on $CuInS_2$ chalcopyrite; in RG 1)
- 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)
- Nippon Steel Corporation, Chiba, Japan: “Optimization of steel microstructures on a mesoscopic scale” (in RG 4)
- ODERSUN AG, Frankfurt/Oder: “Modellierung und Simulation von $CuInS_2$-Dünnschicht-Bandsolarzellen (CISCuT) und Modulstrukturen” (Modeling and simulation of the $CuInS_2$ thin-film band solar cells (CISCuT) and of the modul structures; in RG 1)
- 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 Open Grid Europe GmbH Essen; in RG 4)

A.3 Membership in Editorial Boards[2]

1. P. Friz, Editorial Board, Monatshefte der Mathematik, Springer-Verlag, Berlin.
2. ———, Editorial Board, Annals of Applied Probability, Institute of Mathematical Statistics (IMS), Beachwood, Ohio, USA.
3. G. Blanchard, Editorial Board, Annales de l'Institut Henri Poincaré, Probabilités et Statistiques, Institute of Mathematical Statistics (IMS), Beachwood, Ohio, USA.
4. ———, Editorial Board, Electronic Journal of Statistics, Institute of Mathematical Statistics (IMS), Beachwood, Ohio, USA.
5. R. Henrion, Editorial Board, Nonlinear Analysis: Theory, Methods & Applications, Elsevier, Amsterdam, The Netherlands.
6. ———, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Dordrecht, The Netherlands.
7. ———, Editorial Board, International Journal of Management Science and Engineering Management (MSEM), World Academic Press, Liverpool, UK.
8. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
9. W. König, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
10. V. Krätschmer, Editorial Board, Applied Computational Intelligence and Soft Computing, Hindawi Publishing Corporation, New York, USA.
11. P. Mathé, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
12. ———, Editorial Board, Journal of Complexity, Elsevier, Amsterdam, The Netherlands.
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. ———, Editorial Board, Archive for Rational Mechanics and Analysis, Springer-Verlag, Berlin, Heidelberg.
16. ———, Editorial Board, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
17. ———, Editorial Board, European Series in Applied and Industrial Mathematics: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
18. ———, Editorial Board, Mathematical Models and Methods in Applied Sciences, Imperial College Press, London, UK.
19. ———, Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
20. H. Neidhardt, Editorial Board, Nanosystems: Physics, Chemistry, Mathematics, St. Petersburg State University of Information Technologies, Mechanics and Optics, Russia.
21. ———, Editorial Board, Advances in Mathematical Physics, Hindawi Publishing Corporation, New York, USA.
22. J. Polzehl, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.
23. ———, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, The Netherlands.

[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. J.G.M. Schoenmakers, Editorial Board, Journal of Computational Finance, Incisive Media Investments Limited, London, UK.
25. ———, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
26. J. Sprekels, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.
27. ———, Editorial Board, Mathematics and its Applications, Annals of the Academy of Romanian Scientists, Academy of Romanian Scientists, Bucharest, Romania.
28. ———, Editor, Advances in Mathematical Sciences and Applications, Gakkōtosho, Tokyo, Japan.
29. W. Wagner, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.

A.4 Conferences, Colloquia, and Workshops

A.4.1 WIAS Conferences, Colloquia, and Workshops

Workshop on Drift-Diffusion Systems and Related Problems: Analysis, Algorithms and Computations
Berlin, March 25
Organized by: WIAS (RG 3 and LG 1)

Drift-diffusion systems and related problems constitute a significant problem class with high relevance in applications like semiconductor devices, porous media flow, and electrochemistry. Their appropriate numerical treatment, especially in three space dimensions, still is subject to challenges in many fields of numerical analysis. These challenges include the development and analysis of mathematical models, appropriate discretizations, which conserve important qualitative properties, efficient and accurate solvers, and the construction of appropriate discretization meshes. During the workshop, distinguished speakers from these different fields provided insight into their past and present activities and discussed new challenges for future research. There were 34 participants in the workshop.

6th Singular Days on Asymptotic Methods for PDEs
Berlin, April 29 – May 1, 2010
Organized by: WIAS (RG 1 and LG 2)
Supported by: DFG, WIAS

Partial differential equations (PDEs) play a fundamental role in science and engineering. In real applications, these equations typically have nonsmooth coefficients and are formulated on nonsmooth domains. Furthermore, very thin inclusions or layers have to be taken into account, which have different physical properties than the surrounding material. All these physical and geometric peculiarities may cause singularities in the solutions of the PDEs, which in turn have a strong influence on the convergence rates of numerical schemes. The lectures focused on regularity results for elliptic and parabolic PDEs on nonsmooth domains and with nonsmooth coefficients, on suitably adapted numerical methods, and on applications in physics and mechanics.

For the first time, the international workshop series *Singular Days* took place in Germany. About 50 scientists participated in the workshop. Three key-note lectures, twenty-one talks, and several posters were presented.

Validation in Statistics and Machine Learning
Berlin, October 6–7
Organized by: WIAS (RG 6), Ludwigs-Maximilians-Universität (LMU) München
Supported by: WIAS, PASCAL2 European Network of Excellence

In statistics and machine learning, the evaluation of algorithms typically relies on their performance on data. This is because, in contrast to a theoretical guarantee (e.g., a consistency result), it is in general not possible to prove that an algorithm performs well on a particular (unseen) data set. Therefore, it is of vital importance to ensure the reliability of data-based evaluations. This requirement poses a wide range of open research problems and challenges.

These included:

- the lack of a ground truth to validate results in real-world applications
- the high instability of empirical results in many settings
- the difficulty to make statistics and machine learning research reproducible
- the general over-optimism of published research findings due to pre-publication optimization of the algorithms and publication bias

This workshop—organized by Nicole Krämer (WIAS) and Anne-Laure Boulesteix (LMU Munich)—brought together 49 scientists from statistics, machine learning, and their application fields. The workshop featured 13

invited talks, three contributed talks, and eight contributed poster presentations. It served as a platform to critically discuss current shortcomings, to exchange new approaches, and to identify promising future directions of research.

Localized Structures in Dissipative Nonlinear Systems
Berlin, October 18–20, 2010
Organized by: WIAS (RG 2), Matheon Project Group D14 "Nonlocal and nonlinear effects in fiber optics"
Supported by: DFG Research Center Matheon, WIAS

The aim of the workshop was to bring together a worldwide community of researchers working in the field of theoretical and experimental studies of nonlinear systems that exhibit self-organized dissipative structures. Particular attention was paid to the spatially and temporally localized structures of light in active and passive nonlinear optical systems, the so-called *optical dissipative solitons*. A wide spectrum of topics concerning formation, properties, and applications of dissipative and conservative optical solitons was covered:

- cavity solitons in active and passive optical systems
- stability, control, interaction, and mobility properties of dissipative solitons
- generation and propagation of pulses in optical fibers and waveguide arrays
- optical solitons in nonlocal and dispersive media

The workshop had 36 participants from 12 countries worldwide, including 23 invited speakers who were internationally recognized leading experts in the fields of nonlinear dynamics in optical systems, soliton theory, and pattern formation.

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

Distinguished Lecture Series: 200 Years of Finance and Statistics
Berlin, January 29–30
Organized by: WIAS (RG 6), SFB 649 "Economic Risk", C.A.S.E. — Center for Applied Statistics and Economics (Humboldt-Universität zu Berlin)
Supported by: WIAS, Humboldt-Universität zu Berlin

In 2010, the Humboldt-Universität zu Berlin celebrated its 200th anniversary. To mark this event, C.A.S.E. and the Collaborative Research Center (SFB) 649 in cooperation with the Weierstrass Institute organized the "Distinguished Lecture Series: 200 Years of Finance and Statistics" at the School of Business and Economics, in the Heilig-Geist-Kapelle.

It was a great pleasure to have six Alexander von Humboldt Research Award winners as invited speakers at this symposium:

- Raymond Carroll, Texas A&M University: "Generalized functional linear models with semiparametric single-index interactions"
- Francis Diebold, University of Pennsylvania: "Yield curve modeling and forecasting: Retrospect and prospect"
- Jianqing Fan, Princeton University: "Portfolio allocation and risk assessment using high-frequency data"
- Joel Horowitz, Northwestern University: "Nonparametric instrumental variables estimation"
- Ya'acov Ritov, The Hebrew University of Jerusalem: "From statistical induction and deduction to transduction"
- Stephen Stigler, University of Chicago: "Some historical reflections on risk, speculation and statistics"

The event was attended by more than 100 participants from many countries and included seven invited talks. The major topics were:

– Statistics
– Econometrics
– Finance

μTOSS 2010 Berlin — Multiple Comparisons from Theory to Practice
Berlin, February 15–16
Organized by: Technische Universität (TU) Berlin, WIAS (RG 6), BFNT-B (Bernstein Focus: Neurotechnology Berlin)
Supported by: PASCAL2 European Network of Excellence, TU Berlin, WIAS

The workshop was a success, with a series of high quality talks including keynotes and introductory presentations of "founding fathers" of the field of multiple testing/multiple comparisons (Y. Benjamini, E. Brunner, H. Finner) and accounts of very recent developments (such as presentations by A. Célisse, M. Posch, D. Yekutieli, J. Goeman). A poster session was also organized. Several slots were used to present the outcome of the PASCAL2 (Pattern Analysis, Statistical Modelling and Computational Learning) μTOSS harvest programme project.

There were 23 registered attendants (in addition to the presenters themselves and the members of the μTOSS project, so in total 40 participants), nine plenary talks, and about a dozen poster contributions.

9th German Open Conference on Probability and Statistics ("Leipziger Stochastik-Tage 2010")
Universität Leipzig, March 2–5
Organized by: WIAS (RG 5), The Probability & Statistics Group of DMV
Supported by: Universität Leipzig, DFG, various publishers

Wolfgang König, head of WIAS's Research Group *Interacting Random Systems*, chaired the Local Organizing Committee.

"Leipziger Stochastik-Tage" is the biannual meeting of the Probability & Statistics Group of DFG, which takes place in different German cities (2008: Aachen, 2006: Frankfurt, etc.). Four plenary and 15 main session speakers were invited, and additional 300 contributed talks were given. About 450 participants took part, half of them from Germany, and about 10 percent from overseas. The workshop covered all topics in Probability and Statistics; the 15 sessions took place simultaneously.

Workshop on Random Media in celebration of Jürgen Gärtner's 60th birthday
Technische Universität (TU) Berlin, April 8–10
Organized by: WIAS (RG 5), DFG Research Unit FOR 718 "Analysis and Stochastics in Complex Physical Systems"
Supported by: DFG (FOR 718), Deutsche Bank Qualitative Products Laboratory, TU Berlin

The main subjects of this workshop were random walks in random media, intermittency effects, the parabolic Anderson model, and branching processes. There were about 15 speakers invited from all over the world, mostly former and current co-workers of Jürgen Gärtner, among them Frank den Hollander, Mark Freidlin, Alain-Sol Sznitman, Erwin Bolthausen, and Don Dawson. The workshop was attended by about 50 participants from 15 countries.

XVII International ISIMM Conference on Trends in Applications of Mathematics to Mechanics (STAMM 2010)
Berlin, August 30 – September 2, 2010
Organized by: WIAS (RG 1), Technische Universität (TU) Berlin
Supported by: DFG, TU Berlin, WIAS, DFG Research Center Matheon

The *Symposia on Trends of Applications of Mathematics to Mechanics* (STAMM) are a bi-annual conference series, organized under the auspices of the International Society for the Interaction of Mathematics and Mechanics. The 17 th STAMM conference was held in Schmöckwitz near Berlin and organized jointly by Professors Wolfgang Müller (TU Berlin) and Alexander Mielke (WIAS). About 50 top international scientists from mechanics,

physics, and mathematics gathered to discuss frontier research. September 1, 2010, was devoted to a *Special Ericksen Session* to honor the first awardee of the newly established *ISIMM Prize* for outstanding achievements in interaction of mathematics and mechancis.

Workshop on Probabilistic Techniques in Statistical Mechanics celebrating the 65th birthday of Erwin Bolthausen (University of Zurich)
Technische Universität (TU) Berlin, October 14–16
Organized by: WIAS (RG 5), DFG Research Unit FOR 718 "Analysis and Stochastics in Complex Physical Systems"
Supported by: DFG (FOR 718, IRTG "Stochastic Models of Complex Processes"), TU Berlin, Springer-Verlag

This workshop concentrated on the topics studied by Erwin Bolthausen (who was a professor at TU Berlin from 1979–1990): spin glass models, self-interacting random walks, interacting polymer models, large deviations. About 20 speakers from all over the world were invited, among them Wendelin Werner, Frank den Hollander, Ofer Zeitouni, Amir Dembo, and Gerard Ben Arous. About 80 participants attended the talks.

A.5 Membership in Organizing Committees of non-WIAS Meetings[3]

1. P. Friz, co-organizer, *Advanced Mathematical Methods for Finance*, Humboldt-Universität zu Berlin and Technische Universität Berlin, September 27–30.
2. U. Bandelow, member of the Program Committee, *10th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD) 2010*, Georgia Institute of Technology, Atlanta, USA, September 6–9.
3. D. Hömberg, member of the Scientific Committee, *Warsaw Seminar on Industrial Mathematics (WSIM'10)*, Warsaw University of Technology, Poland, March 18–19.
4. V. John, organizer, *Colloquium on the Occasion of Prof. Lutz Tobiska's 60th Birthday*, Otto-von-Guericke-Universität Magdeburg, December 3.
5. W. König, organizer, *Berlin-Leipzig Seminar on Analysis and Probability Theory*, Rheinische Friedrich-Wilhelms-Universität Bonn, January 15.
6. ———, chair of the Local Organizing Committee, *9th German Open Conference on Probability and Statistics*, Universität Leipzig, March 2–5.
7. ———, member of the Program Committee, *Workshop on Random Media in Celebration of Jürgen Gärtner's 60th Birthday*, Technische Universität Berlin, April 8–10.
8. ———, organizer, *Berlin-Leipzig Seminar on Analysis and Probability Theory*, Universität Heidelberg, June 18.
9. ———, organizer, *Berlin-Leipzig Seminar on Analysis and Probability Theory*, Technische Universität Berlin, July 9.
10. ———, member of the Program Committee, *Workshop on Probabilistic Techniques in Statistical Mechanics in Celebration of Erwin Bolthausen's 65th Birthday*, Technische Universität Berlin, October 14–16.
11. ———, organizer, *Berlin-Leipzig Seminar on Analysis and Probability Theory*, Max-Planck-Institut für Mathematik in den Naturwissenschaften, November 26.
12. A. Mielke, co-organizer, *Workshop "Microstructures in Solids: From Quantum Models to Continua"*, Mathematisches Forschungsinstitut Oberwolfach, March 15–19.
13. M. Radziunas, member of the International Scientific Committee, *15th International Conference "Mathematical Modelling and Analysis" (MMA2010)*, Druskininkai, Lithuania, May 26–29.
14. V. Spokoiny, organizer, *Workshop "Modern Nonparametric Statistics: Going Beyond Asymptotic Minimax"*, Mathematisches Forschungsinstitut Oberwolfach, March 29 – April 2.
15. B. Wagner, organizer of the minisymposium "MS84: Dynamics of Thin Films of Complex Liquids" (together with A. Münch), *SIAM Conference on Mathematical Aspects of Materials Science (MS10)*, Philadelphia, USA, May 22–26.
16. M. Wolfrum, member of the Scientific Committee, *International Workshop "Nonlinear Dynamics on Networks"*, National Academy of Sciences of Ukraine, Kiev, July 5–9.

[3] Memberships in organizing committees of non-WIAS meetings by guests during their long-term stay at WIAS have been listed in front of those by the collaborators of WIAS.

A.6 Publications[4]

A.6.1 Monographs

[1] P. Friz, N.B. Victoir, *Multidimensional Stochastic Processes as Rough Paths*, vol. 120 of Cambridge Studies in Advanced Mathematics, Cambridge University Press, Cambridge, 2010, 670 pages.

A.6.2 Editorship of Proceedings and Collected Editions

[1] B. Wagner, B. Rech, A. Münch, V. Mehrmann, eds., *Proceedings of the Workshop Mathematics in Industry: Technologies of Thin Film Solar Cells*, WIAS, Berlin, 2010, 68 pages.

A.6.3 Outstanding Contributions to Monographs

[1] W. Dreyer, *Production and Use of Novel Materials, in: Production Factor Mathematics*, M. Grötschel, K. Lucas, V. Mehrmann, eds., Springer, Berlin/Heidelberg, 2010, pp. 249–262.

Outstanding Contributions to Monographs (to appear)

[1] O. Schenk, K. Gärtner, *PARDISO, in: Encyclopedia of Parallel Computing*, Springer.

A.6.4 Articles in Refereed Journals

[1] P. Friz, Th. Cass, *Densities for rough differential equations under Hoermander's condition*, Ann. Math. (2), 171 (2010), pp. 2115–2141.

[2] P. Friz, H. Oberhauser, *A generalized Fernique theorem and applications*, Proc. Amer. Math. Soc., 138 (2010), pp. 3679–3688.

[3] P. Friz, N. Victoir, *Differential equations driven by Gaussian signals*, Ann. Inst. H. Poincare Probab. Statist., 46 (2010), pp. 369–413.

[4] S. Amiranashvili, U. Bandelow, A. Mielke, *Padé approximant for refractive index and nonlocal envelope equations*, Opt. Commun., 283 (2010), pp. 480–485.

[5] S. Amiranashvili, A. Demircan, *Hamiltonian structure of propagation equations for ultrashort optical pulses*, Phys. Rev. A, 82 (2010), pp. 013812/1–013812/11.

[6] H.-G. Purwins, H. Bödeker, S. Amiranashvili, *Dissipative solitons*, Adv. Phys., 59 (2010), pp. 485–701.

[7] S. Amiranashvili, A.G. Vladimirov, U. Bandelow, *A model equation for ultrashort optical pulses around the zero dispersion frequency*, Eur. Phys. J. D, 58 (2010), pp. 219–226.

[8] I. Babushkin, *Non-Poissonian statistics in an optical analog of quantum billiard with perfectly square boundaries*, Phys. Lett. A, 374 (2010), pp. 896–900.

[9] I. Babushkin, W. Kuehn, Ch. Köhler, St. Skupin, L. Bergé, K. Reimann, M. Woerner, J. Herrmann, Th. Elsaesser, *Ultrafast spatio-temporal dynamics of terahertz generation by ionizing two-color femtosecond pulses in gases*, Phys. Rev. Lett., 105 (2010), pp. 053903/1–053903/4.

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

[10] 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*, Phys. Rev. A, 81 (2010), pp. 023819/1–023819/11.

[11] I. Babushkin, St. Skupin, J. Herrmann, *Generation of terahertz radiation from ionizing two-color laser pulses in Ar filled metallic hollow waveguides*, Optics Express, 18 (2010), pp. 9658–9663.

[12] D. Belomestny, *Spectral estimation of the fractional order of a Lévy process*, Ann. Statist., 38 (2010), pp. 317–351.

[13] D. Belomestny, L. Rüschendorf, M. Urusov, *Optimal stopping of integral functionals and a "no-loss" free boundary formulation*, SIAM J. Theory Probab. Appl., 54 (2010), pp. 14–28.

[14] D. Belomestny, A. Kolodko, J.G.M. Schoenmakers, *Pricing CMS spreads in the Libor market model*, Int. J. Theor. Appl. Finance, 13 (2010), pp. 45–62.

[15] ———, *Regression methods for stochastic control problems and their convergence analysis*, SIAM J. Control Optim., 48 (2010), pp. 3562–3588.

[16] D. Belomestny, G.N. Milstein, J.G.M. Schoenmakers, *Sensitivities for Bermudan options by regression methods*, Decis. Econ. Finance, 33 (2010), pp. 117–138.

[17] G. Blanchard, *Adaptive FDR control under independence and dependence*, J. Mach. Learn. Res., 10 (2010), pp. 2837–2871.

[18] S. Arlot, G. Blanchard, E. Roquain, *Some non-asymptotic results on resampling in high dimension, I: Confidence regions*, Ann. Statist., 38 (2010), pp. 51–82.

[19] ———, *Some non-asymptotic results on resampling in high dimension, II: Multiple tests*, Ann. Statist., 38 (2010), pp. 83–99.

[20] G. Blanchard, G. Lee, C. Scott, *Semi-supervised novelty detection*, J. Mach. Learn. Res., 11 (2010), pp. 2973–3009.

[21] G. Blanchard, P. Mathé, *Conjugate gradient regularization under general smoothness and noise assumptions*, J. Inverse Ill-Posed Probl., 18 (2010), pp. 701–726.

[22] C. Bréé, J. Bethge, St. Skupin, L. Bergé, A. Demircan, G. Steinmeyer, *Cascaded self-compression of femtosecond pulses in filaments*, New J. Phys., 12 (2010), pp. 093046/1–093046/11.

[23] C. Bréé, A. Demircan, St. Skupin, L. Bergé, G. Steinmeyer, *Plasma induced pulse breaking in filamentary self-compression*, Laser Physics, 20 (2010), pp. 1107–1113.

[24] C. Bréé, A. Demircan, G. Steinmeyer, *Method for computing the nonlinear refractive index via Keldysh theory*, IEEE J. Quantum Electron., 46 (2010), pp. 433–437.

[25] E. Diederichs, A. Juditsky, V. Spokoiny, Ch. Schütte, *Sparse non-Gaussian component analysis*, IEEE Trans. Inform. Theory, 56 (2010), pp. 3033–3047.

[26] W. Dreyer, J. Jamnik, C. Guhlke, R. Huth, J. Moškon, M. Gaberšček, *The thermodynamic origin of hysteresis in insertion batteries*, Nature Materials, 9 (2010), pp. 448–453.

[27] W. Dreyer, Ch. Kraus, *On the van der Waals–Cahn–Hilliard phase-field model and its equilibria conditions in the sharp interface limit*, Proc. Roy. Soc. Edinburgh Sect. A, 140 A (2010), pp. 1161–1186.

[28] P.-É. Druet, *Weak solutions to a time-dependent heat equation with nonlocal radiation boundary condition and arbitrary p-summable right-hand side*, Appl. Math., 55 (2010), pp. 111–149.

[29] J. Elschner, M. Yamamoto, *Uniqueness in inverse elastic scattering with finitely many incident waves*, Inverse Problems, 26 (2010), pp. 045005/1–045005/8.

[30] S. Chandler-Wilde, J. Elschner, *Variational approach in weighted Sobolev spaces to scattering by unbounded rough surface*, SIAM J. Math. Anal., 42 (2010), pp. 2554–2580.

[31] J. Elschner, G. Hu, *Global uniqueness in determining polygonal periodic structures with a minimal number of incident plane waves*, Inverse Problems, 26 (2010), pp. 115002/1–115002/23.

[32] ———, *Variational approach to scattering of plane elastic waves by diffraction gratings*, Math. Methods Appl. Sci., 33 (2010), pp. 1924–1941.

[33] J. Fuhrmann, A. Bradji, *Error estimates of the discretization of linear parabolic equations on general nonconforming spatial grids*, C. R. Math. Acad. Sci. Paris, 348 (2010), pp. 1119–1122.

[34] J. Fuhrmann, A. Fiebach, A. Erdmann, P. Trefonas, *Acid diffusion effects between resists in freezing processes used for contact hole patterning*, Microel. Engineering, 87 (2010), pp. 951–954.

[35] J. Becker, K. Gärtner, R. Klanner, R. Richter, *Simulation and experimental study of plasma effects in planar silicon sensors*, Nucl. Inst. Meth. Phys. Research A, 624 (2010), pp. 716–727.

[36] L. Strüder, S. Epp, K. Gärtner, J. Ullrich, et al., *Large-format, high-speed, X-ray pnCCDs combined with electron and ion imaging spectrometers in a multipurpose chamber for experiments at 4th generation light sources*, Nucl. Inst. Meth. Phys. Research A, 614 (2010), pp. 483–496.

[37] A. Glitzky, K. Gärtner, *Existence of bounded steady state solutions to spin-polarized drift-diffusion systems*, SIAM J. Math. Anal., 41 (2010), pp. 2489–2513.

[38] A. Glitzky, J.A. Griepentrog, *Discrete Sobolev–Poincaré inequalities for Voronoi finite volume approximations*, SIAM J. Numer. Anal., 48 (2010), pp. 372–391.

[39] J.A. Griepentrog, L. Recke, *Local existence, uniqueness, and smooth dependence for nonsmooth quasilinear parabolic problems*, J. Evol. Equ., 10 (2010), pp. 341–375.

[40] L. Andrieu, R. Henrion, W. Römisch, *A model for dynamic chance constraints in hydro power reservoir management*, European J. Oper. Res., 207 (2010), pp. 579–589.

[41] M.J. Fabian, R. Henrion, A.Y. Kruger, J. Outrata, *Error bounds: Necessary and sufficient conditions*, Set-Valued Var. Anal., 18 (2010), pp. 121–149.

[42] R. Henrion, B. Mordukhovich, N.M. Nam, *Second-order analysis of polyhedral systems in finite and infinite dimensions with applications to robust stability of variational inequalities*, SIAM J. Optim., 20 (2010), pp. 2199–2227.

[43] R. Henrion, J. Outrata, Th. Surowiec, *A note on the relation between strong and M-stationarity for a class of mathematical programs with equilibrium constraints*, Kybernetika, 46 (2010), pp. 423–434.

[44] R. Henrion, W. Römisch, *Lipschitz and differentiability properties of quasi-concave and singular normal distribution functions*, Ann. Oper. Res., 177 (2010), pp. 115–125.

[45] R. Henrion, A. Seeger, *Inradius and circumradius of various convex cones arising in applications*, Set-Valued Var. Anal., 18 (2010), pp. 483–511.

[46] ———, *On properties of different notions of centers for convex cones*, Set-Valued Var. Anal., 18 (2010), pp. 205–231.

[47] W. van Ackooij, R. Henrion, A. Möller, R. Zorgati, *On probabilistic constraints induced by rectangular sets and multivariate normal distributions*, Math. Methods Oper. Res., 71 (2010), pp. 535–549.

[48] A. Fasano, D. Hömberg, D. Naumov, *On a mathematical model for laser-induced thermotherapy*, Appl. Math. Modelling, 34 (2010), pp. 3831–3840.

[49] D. Hömberg, Ch. Meyer, J. Rehberg, W. Ring, *Optimal control for the thermistor problem*, SIAM J. Control Optim., 48 (2010), pp. 3449–3481.

[50] G. Hu, F. Qu, B. Zhang, *Direct and inverse problems for electromagnetic scattering by a doubly periodic structure with a partially coated dielectric*, Math. Methods Appl. Sci., 33 (2010), pp. 147–156.

[51] X. Liu, B. Zhang, G. Hu, *Uniqueness in the inverse scattering problem in a piecewise homogeneous medium*, Inverse Problems, 26 (2010), pp. 015002/1–015002/14.

[52] M. Aizenman, S. Jansen, P. Jung, *Symmetry breaking in quasi-1D Coulomb systems*, Ann. Henri Poincare, 11 (2010), pp. 1453–1485.

[53] L.G.M. de Souza, G. Janiga, V. John, D. Thévenin, *Reconstruction of a distribution from a finite number of moments with an adaptive spline-based algorithm*, Chem. Engng. Sci., 65 (2010), pp. 2741–2750.

[54] V. John, A. Kindl, *Numerical studies of finite element variational multiscale methods for turbulent flow simulations*, Comput. Methods Appl. Mech. Engrg., 199 (2010), pp. 841–852.

[55] ———, *A variational multiscale method for turbulent flow simulation with adaptive large scale space*, J. Comput. Phys., 229 (2010), pp. 301–312.

[56] V. John, J. Rang, *Adaptive time step control for the incompressible Navier–Stokes equations*, Comput. Methods Appl. Mech. Engrg., 199 (2010), pp. 514–524.

[57] V. John, M. Roland, *On the impact of the scheme for solving the higher-dimensional equation in coupled population balance systems*, Internat. J. Numer. Methods Engrg., 82 (2010), pp. 1450–1474.

[58] V. John, A. Kindl, O.C. Suciu, *Finite element LES and VMS methods on tetrahedral meshes*, J. Comput. Appl. Math., (2010), pp. 3095–3102.

[59] H.-Chr. Kaiser, J. Rehberg, *Optimal elliptic regularity at the crossing of a material interface and a Neumann boundary edge*, J. Math. Sci. (N. Y.), 169 (2010), pp. 145–166.

[60] G. Kitavtsev, B. Wagner, *Coarsening dynamics of slipping droplets*, J. Engrg. Math., 66 (2010), pp. 271–292.

[61] D. Knees, *On global spatial regularity and convergence rates for time dependent elasto-plasticity*, Math. Models Methods Appl. Sci., 20 (2010), pp. 1823–1858.

[62] D. Knees, Ch. Zanini, A. Mielke, *Crack growth in polyconvex materials*, Phys. D, 239 (2010), pp. 1470–1484.

[63] P. Gruber, D. Knees, S. Nesenenko, M. Thomas, *Analytical and numerical aspects of time-dependent models with internal variables*, ZAMM Z. Angew. Math. Mech., 90 (2010), pp. 861–902.

[64] A. Collevecchio, W. König, P. Mörters, N. Sidorova, *Phase transitions for dilute particle systems with Lennard–Jones potential*, Comm. Math. Phys., 299 (2010), pp. 603–630.

[65] W. König, P. Schmid, *Random walks conditioned to stay in Weyl chambers of type C and D*, Electron. Comm. Probab., (2010), pp. 286–295.

[66] M.D. Korzec, P. Evans, *From bell shapes to pyramids: A reduced continuum model for self-assembled quantum dot growth*, Phys. D, 239 (2010), pp. 465–474.

[67] V. Krätschmer, J.G.M. Schoenmakers, *Representations for optimal stopping under dynamic monetary utility functionals*, SIAM J. Financial Math., 1 (2010), pp. 811–832.

[68] H. Garcke, Ch. Kraus, *An anisotropic, inhomogeneous, elastically modified Gibbs–Thomson law as singular limit of a diffuse interface model*, Adv. Math. Sci. Appl., 20 (2010), pp. 511–545.

[69] K. Krumbiegel, Ch. Meyer, A. Rösch, *A priori error analysis for linear quadratic elliptic Neumann boundary control problems with control and state constraints*, SIAM J. Control Optim., 48 (2010), pp. 5108–5142.

[70] K. Krumbiegel, I. Neitzel, A. Rösch, *Sufficient optimality conditions for the Moreau–Yosida-type regularization concept applied to semilinear elliptic optimal control problems with pointwise state constraints*, Ann. Acad. Rom. Sci. Math. Appl., 2 (2010), pp. 222–246.

[71] A. Caboussat, Ch. Landry, J. Rappaz, *Optimization problem coupled with differential equations: A numerical algorithm mixing an interior-point method and event detection*, J. Optim. Theory Appl., 147 (2010), pp. 141–156.

[72] A.L. Bowers, B.R. Cousins, A. Linke, L.G. Rebholz, *New connections between finite element formulations of the Navier–Stokes equations*, J. Comput. Phys., 229 (2010), pp. 9020–9025.

[73] J. Härdtlein, C. Pflaum, A. Linke, C.H. Wolters, *Advanced expression templates programming*, Comput. Vis. Sci., 13 (2010), pp. 59–68.

[74] R.L. Loeffen, J.-F. Renaud, *De Finetti's optimal dividends problem with an affine penalty function at ruin*, Insurance Math. Econom., 46 (2010), pp. 98–108.

[75] A.E. Kyprianou, R.L. Loeffen, *Refracted Lévy processes*, Ann. Inst. H. Poincare Probab. Statist., 46 (2010), pp. 24–44.

[76] J. Giannoulis, A. Mielke, Ch. Sparber, *High-frequency averaging in semi-classical Hartree-type equations*, Asymptot. Anal., 70 (2010), pp. 87–100.

[77] A. Mielke, C. Patz, *Dispersive stability of infinite dimensional Hamiltonian systems on lattices*, Appl. Anal., 89 (2010), pp. 1493–1512.

[78] A. Mielke, T. Roubíček, J. Zeman, *Complete damage in elastic and viscoelastic media and its energetics*, Comput. Methods Appl. Mech. Engrg., 199 (2010), pp. 1242–1253.

[79] A. Mielke, L. Paoli, A. Petrov, U. Stefanelli, *Error estimates for space-time discretizations of a rate-independent variational inequality*, SIAM J. Numer. Anal., 48 (2010), pp. 1625–1646.

[80] S. Bartels, R. Müller, *A posteriori error controlled local resolution of evolving interfaces for generalized Cahn–Hilliard equations*, Interfaces Free Bound., 12 (2010), pp. 45–73.

[81] M.M. Malamud, H. Neidhardt, *On Kato–Rosenblum and Weyl–von Neumann theorems*, Dokl. Akad. Nauk, 432 (2010), pp. 161–166.

[82] O.E. Omel'chenko, Y.L. Maistrenko, P.A. Tass, *Chimera states induced by spatially modulated delayed feedback*, Phys. Rev. E (3), 82 (2010), pp. 066201/1–066201/13.

[83] O.E. Omel'chenko, M. Wolfrum, Y.L. Maistrenko, *Chimera states as chaotic spatio-temporal patterns*, Phys. Rev. E (3), 81 (2010), pp. 065201/1–065201/4.

[84] D. Peschka, A. Münch, B. Niethammer, *Self-similar rupture of viscous thin films in the strong-slip regime*, Nonlinearity, 23 (2010), pp. 409–427.

[85] ———, *Thin film rupture for large slip*, J. Engrg. Math., 66 (2010), pp. 33–51.

[86] J. Polzehl, H.U. Voss, K. Tabelow, *Structural adaptive segmentation for statistical parametric mapping*, NeuroImage, 52 (2010), pp. 515–523.

[87] R. Racec, U. Wulf, P.N. Racec, *Fano regime of transport through open quantum dots*, Phys. Rev. B., 82 (2010), pp. 085313/1–085313/16.

[88] R. Čiegis, M. Radziunas, *Effective numerical integration of traveling wave model for edge-emitting broad-area semiconductor lasers and amplifiers*, Math. Model. Anal., 15 (2010), pp. 409–430.

[89] H. Gross, J. Richter, A. Rathsfeld, M. Bär, *Investigations on a robust profile model for the reconstruction of 2D periodic absorber lines in scatterometry*, J. Eur. Opt. Soc. Rapid Publ., 5 (2010), pp. 10053/1–10053/7.

[90] R. Haller-Dintelmann, J. Rehberg, *Coercivity for elliptic operators and positivity of solutions on Lipschitz domains*, Arch. Math. (Basel), 95 (2010), pp. 457–468.

[91] L.I. Goray, G. Schmidt, *Solving conical diffraction grating problems with integral equations*, J. Opt. Soc. Amer. A, 27 (2010), pp. 585–597.

[92] N. Serdyukova, *Dependence on the dimension for complexity of approximation of random fields*, Theory Probab. Appl., 54 (2010), pp. 272–284.

[93] H. Si, *Constrained Delaunay tetrahedral mesh generation and refinement*, Finite Elem. Anal. Des., 46 (2010), pp. 33–46.

[94] H. Si, J. Fuhrmann, K. Gärtner, *Boundary conforming Delaunay mesh generation*, Comput. Math. Math. Phys., 50 (2010), pp. 38–53.

[95] Y. Chen, W. Härdle, V. Spokoiny, *GHICA — Risk analysis with GH distributions and independent components*, J. Empirical Finance, 17 (2010), pp. 255–269.

[96] J. Sprekels, H. Wu, *A note on parabolic equation with nonlinear dynamical boundary condition*, Nonlinear Anal., 72 (2010), pp. 3028–3048.

[97] P. Colli, G. Gilardi, P. Podio-Guidugli, J. Sprekels, *Existence and uniqueness of a global-in-time solution to a phase segregation problem of the Allen–Cahn type*, Math. Models Methods Appl. Sci., 20 (2010), pp. 519–541.

[98] ———, *A temperature-dependent phase segregation problem of the Allen–Cahn type*, Adv. Math. Sci. Appl., 20 (2010), pp. 219–234.

[99] O. Anoshchenko, E. Khruslov, H. Stephan, *Global weak solutions to the Navier–Stokes–Vlasov–Poisson system*, J. Mathematical Physics Analysis Geometry (MAG), 6 (2010), pp. 143–182.

[100] M. Thomas, A. Mielke, *Damage of nonlinearly elastic materials at small strain — Existence and regularity results*, ZAMM Z. Angew. Math. Mech., 90 (2010), pp. 88–112.

[101] P. Suwanpinij, N. Togobytska, U. Prahl, W. Weiss, D. Hömberg, W. Bleck, *Numerical cooling strategy design for hot rolled dual phase steel*, Steel Res. Int., 81 (2010), pp. 1001–1009.

[102] V.Z. Tronciu, *Chaos communication using semiconductor lasers subject to different kinds of optical feedback*, Moldavian J. Phys. Sci., 9 (2010), pp. 50–69.

[103] V.Z. Tronciu, C. Mirasso, P. Colet, M. Hamacher, M. Benedetti, V. Vercesi, V. Annovazzi-Lodi, *Chaos generation and synchronization using an integrated source with an air gap*, IEEE J. Quantum Electron., 46 (2010), pp. 1840–1846.

[104] Ch. Fiebig, V.Z. Tronciu, M. Lichtner, H. Wenzel, K. Paschke, *Experimental and numerical study of distributed Bragg reflector tapered lasers*, Appl. Phys. B, 99 (2010), pp. 209–214.

[105] M. Tlidi, A.G. Vladimirov, D. Turaev, G. Kozyreff, D. Pieroux, T. Erneux, *Spontaneous motion of localized structures and localized patterns induced by delayed feedback*, Eur. Phys. J. D, 59 (2010), pp. 59–65.

[106] A.G. Vladimirov, U. Bandelow, G. Fiol, D. Arsenijević, M. Kleinert, D. Bimberg, A. Pimenov, D. Rachinskii, *Dynamical regimes in a monolithic passively mode-locked quantum dot laser*, J. Opt. Soc. Amer. B Opt. Phys., 27 (2010), pp. 2102–2109.

[107] G. Fiol, D. Arsenijević, D. Bimberg, A.G. Vladimirov, M. Wolfrum, E.A. Viktorov, P. Mandel, *Hybrid mode-locking in a 40 GHz monolithic quantum dot laser*, Appl. Phys. Lett., 96 (2010), pp. 011104/1–011104/3.

[108] W. Wagner, *Random and deterministic fragmentation models*, Monte Carlo Methods Appl., 16 (2010), pp. 399–420.

[109] A. Braumann, M. Kraft, W. Wagner, *Numerical study of a stochastic particle algorithm solving a multidimensional population balance model for high shear granulation*, J. Comput. Phys., 229 (2010), pp. 7672–7691.

[110] O. Muscato, V. Di Stefano, W. Wagner, *Numerical study of the systematic error in Monte Carlo schemes for semiconductors*, ESAIM Math. Model. Numer. Anal., 44 (2010), pp. 1049–1068.

[111] J.-E. Kim, E. Malic, M. Richter, A. Wilms, A. Knorr, *Maxwell–Bloch equation approach for describing the microscopic dynamics of quantum-dot surface-emitting structures*, IEEE J. Quantum Electron., 46 (2010), pp. 1115–1126.

[112] M.-R. Dachner, E. Malic, M. Richter, A. Carmele, J. Kabuss, A. Wilms, J.-E. Kim, G. Hartmann, J. Wolters, U. Bandelow, A. Knorr, *Theory of carrier and photon dynamics in quantum dot light emitters*, Phys. Status Solidi B, 247 (2010), pp. 809–828.

[113] P. Perlikowski, S. Yanchuk, M. Wolfrum, A. Stefanski, P. Mosiolek, T. Kapitaniak, *Routes to complex dynamics in a ring of unidirectionally coupled systems*, Chaos, 20 (2010), pp. 013111/1–013111/9.

[114] M. Wolfrum, S. Yanchuk, *A multiple time scale approach to the stability of external cavity modes in the Lang–Kobayashi system using the limit of large delay*, SIAM J. Appl. Dyn. Syst., 9 (2010), pp. 519–535.

[115] M. Wolfrum, S. Yanchuk, P. Hövel, E. Schöll, *Complex dynamics in delay-differential equations with large delay*, Eur. Phys. J. D., 191 (2010), pp. 91–103.

[116] M. Wolfrum, O. Omel'chenko, S. Yanchuk, Y. Maistrenko, *Spectral properties of chimera states*, Chaos, 21 (2011), pp. 013112/1–013112/8.

Articles in Refereed Journals (to appear)

[1] M. Beiglboeck, P. Friz, St. Sturm, *Is the minimum value of an option on variance generated by local volatility?*, SIAM J. Financial Math.

[2] M. Caruana, P. Friz, H. Oberhauser, *A (rough) pathwise approach to a class of nonlinear SPDEs*, Ann. Inst. H. Poincare Anal. Non Lineaire.

[3] P. Friz, S. Gerhold, A. Gulisashvili, *On refined volatility smile expansion in the Heston model*, Quant. Finance.

[4] I. Babushkin, U. Bandelow, A.G. Vladimirov, *Rotational symmetry breaking in small-area circular vertical cavity surface emitting lasers*, Opt. Commun.

[5] D. Belomestny, *On the rates of convergence of simulation-based algorithms for optimal stopping problem*, Ann. Appl. Probab.

[6] ———, *Pricing Bermudan options by nonparametric regression: Optimal rates of convergence*, Finance Stoch.

[7] D. Belomestny, P. Gapeev, *An iterative procedure for solving integral equations related to optimal stopping problems*, Stochastics.

[8] D. Belomestny, J.G.M. Schoenmakers, *A jump-diffusion Libor model and its robust calibration*, Quant. Finance.

[9] C. Brée, A. Demircan, G. Steinmeyer, *Modulation instability in filamentary self-compression*, Laser Physics.

[10] A. Caiazzo, D. Evans, J.-L. Falcone, J. Hegewald, E. Lorenz, et al., *A complex automata approach for in-stent restenosis: Two-dimensional multiscale modeling and simulations*, J. Comput. Sci.

[11] A. Caiazzo, M. Fernandez, J.-F. Gerbeau, V. Martin, *Projection schemes for fluid flows through a porous interface*, SIAM J. Sci. Comput.

[12] W. Dreyer, F. Duderstadt, St. Eichler, M. Naldzhieva, *On unwanted nucleation phenomena at the wall of a VGF chamber*, J. Crystal Growth.

[13] W. Dreyer, C. Guhlke, M. Herrmann, *Hysteresis and phase transition in many-particle storage systems*, Contin. Mech. Thermodyn.

[14] W. Dreyer, C. Guhlke, R. Huth, *The behavior of a many particle cathode in a lithium-ion battery*, Phys. D.

[15] W. Dreyer, M. Gaberšček, C. Guhlke, R. Huth, J. Jamnik, *Phase transition and hysteresis in a rechargeable lithium battery revisited*, European J. Appl. Math.

[16] P.-E. Druet, P. Philip, *Noncompactness of integral operators modeling diffuse-gray radiation in polyhedral and transient settings*, Integral Equations Operator Theory.

[17] G. Faraud, *A central limit theorem for random walk in random environment on a marked Galton–Watson tree*, Electron. J. Probab.

[18] J. Fuhrmann, H. Langmach, A. Linke, *A numerical method for mass conservative coupling between fluid flow and solute transport*, Appl. Numer. Math.

[19] A. Glitzky, *Uniform exponential decay of the free energy for Voronoi finite volume discretized reaction-diffusion systems*, Math. Nachr.

[20] H. Hanke, *Homogenization in gradient plasticity*, GAMM-Mitt.

[21] ———, *Homogenization in gradient plasticity*, Math. Models Methods Appl. Sci.

[22] R. Henrion, J. Outrata, Th. Surowiec, *Analysis of M-stationary points to an EPEC modeling oligopolistic competition in an electricity spot market*, ESAIM Control Optim. Calc. Var.

[23] R. Henrion, Th. Surowiec, *On calmness conditions in convex bilevel programming*, Appl. Anal.

[24] W. van Ackooij, R. Henrion, A. Möller, R. Zorgati, *On joint probabilistic constraints with Gaussian coefficient matrix*, Oper. Res. Lett.

[25] K. Chełminski, D. Hömberg, O. Rott, *Mathematical analysis of a thermomechanical milling process*, GAMM-Mitt.

[26] ———, *On a thermomechanical milling model*, Nonlinear Anal. Real World Appl.

[27] G. Hu, J. Yang, B. Zhang, *Inverse electromagnetic scattering for a bi-periodic inhomogeneous layer on perfectly conducting plates*, Appl. Anal.

[28] G. Hu, B. Zhang, *The linear sampling method for the inverse electromagnetic scattering by a partially coated bi-periodic structure*, Math. Methods Appl. Sci.

[29] R. Haller-Dintelmann, H.-Chr. Kaiser, J. Rehberg, *Direct computation of elliptic singularities across anisotropic, multi-material edges*, J. Math. Sci. (N. Y.).

[30] D. Knees, *Global spatial regularity for a regularized elasto-plastic model*, GAMM-Mitt.

[31] St. Adams, A. Collevecchio, W. König, *A variational formula for the free energy of an interacting many-particle system*, Ann. Probab.

[32] K. Krumbiegel, I. Neitzel, A. Rösch, *Regularization error estimates for semilinear elliptic optimal control problems with pointwise state and control constraints*, Comput. Optim. Appl.

[33] M. Spreemann, H. Wenzel, B. Eppich, M. Lichtner, G. Erbert, *Novel approach to finite-aperture tapered unstable resonator lasers*, IEEE J. Quantum Electron.

[34] M. Case, V. Ervin, A. Linke, L. Rebholz, N. Wilson, *Stable computing with an enhanced physics based scheme for the 3D Navier–Stokes equations*, Int. J. Numer. Anal. Model.

[35] F. Bauer, P. Mathé, *Parameter choice methods using minimization schemes*, J. Complexity.

[36] J. Flemming, B. Hofmann, P. Mathé, *Sharp converse results for the regularization error using distance functions*, Inverse Problems.

[37] W. Kirsch, B. Metzger, P. Müller, *Random block operators*, J. Statist. Phys., (2011).

[38] ———, *Random block operators*, J. Statist. Phys., (2011).

[39] A. Mielke, *Complete-damage evolution based on energies and stresses*, Discrete Contin. Dyn. Syst. Ser. S.

[40] ———, *Formulation of thermo-elastic dissipative material behavior using GENERIC*, Contin. Mech. Thermodyn.

[41] ———, *On thermodynamically consistent models and gradient structures for thermoplasticity*, GAMM-Mitt.

[42] A. Mielke, R. Rossi, G. Savaré, *BV solutions and viscosity approximations of rate-independent systems*, ESAIM Control Optim. Calc. Var.

[43] A. Mielke, U. Stefanelli, *Weighted energy-dissipation functionals for gradient flows*, ESAIM Control Optim. Calc. Var.

[44] S. Bartels, R. Müller, Ch. Ortner, *Robust a priori and a posteriori error analysis for the approximation of Allen–Cahn and Ginzburg–Landau equations past topological changes*, SIAM J. Numer. Anal.

[45] S. Bartels, R. Müller, *Quasi-optimal and robust a posteriori error estimates in $L^\infty(L^2)$ for the approximation of Allen–Cahn equations past singularities*, Math. Comp.

[46] P. Exner, H. Neidhardt, V. Zagrebnov, *Remarks on the Trotter–Kato product formula for unitary groups*, Integral Equations Operator Theory.

[47] M.M. Malamud, H. Neidhardt, *On the unitary equivalence of absolutely continuous parts of self-adjoint extensions*, J. Funct. Anal.

[48] K. Kostourou, D. Peschka, A. Münch, B. Wagner, St. Herminghaus, R. Seemann, *Interface morphologies in liquid/liquid dewetting*, Chem. Eng. Proc.

[49] M. Radziunas, A.G. Vladimirov, E.A. Viktorov, G. Fiol, H. Schmeckebier, *Strong pulse asymmetry in quantum-dot mode-locked semiconductor lasers*, Appl. Phys. Lett.

[50] G. Schmidt, *Integral equations for conical diffraction by coated gratings*, J. Integral Equations Appl.

[51] G. Schmidt, B.H. Kleemann, *Integral equation methods from grating theory to photonics: An overview and new approaches for conical diffraction*, J. Modern Opt.

[52] F. Lanzara, V. Maz'ya, G. Schmidt, *On the fast computation of high dimensional volume potentials*, Math. Comp.

[53] J.G.M. Schoenmakers, *A pure martingale dual for multiple stopping*, Finance Stoch.

[54] H. Si, K. Gärtner, *3D boundary recovery by constrained Delaunay tetrahedralization*, Internat. J. Numer. Methods Engrg.

[55] P. Krejčí, E. Rocca, J. Sprekels, *Phase separation in a gravity field*, Discrete Contin. Dyn. Syst. Ser. S.

[56] J. Bardin, J. Fins, D. Katz, J. Hersh, L. Heier, K. Tabelow, J. Dyke, D. Ballon, N. Schiff, H. Voss, *Dissociations between behavioral and fMRI-based evaluations of cognitive function after brain injury*, Brain.

[57] M. Grote, V. Palumberi, B. Wagner, A. Barbero, I. Martin, *Dynamic formation of oriented patches in chondrocyte cell cultures*, J. Math. Biol.

[58] A. Münch, B. Wagner, *Impact of slippage on the morphology and stability of a dewetting rim*, J. Phys.: Condens. Matter.

A.6.5 Contributions to Collected Editions

[1] P. Friz, *Implied volatility: Large strike asymptotics*, in: Encyclopedia of Quantitative Finance, R. Cont, ed., Wiley, Chichester, 2010, pp. 909–913.

[2] P. Friz, M. Keller-Ressel, *Moment explosions in financial models*, in: Encyclopedia of Quantitative Finance, R. Cont, ed., Wiley, Chichester, 2010, pp. 1247–1253.

[3] I. Babushkin, S. Skupin, C. Köhler, L. Bergé, J. Herrmann, *Modeling of THz emission from plasma-generating femtosecond laser pulses with unidirectional Maxwell equation in plasma spots and in guided geometries*, in: Book of Abstracts of the 2nd International Workshop on Laser-Matter Interaction 2010, September 13–17, 2010, Porquerolles, France, 2010, p. 49.

[4] U. Bandelow, Th. Koprucki, A. Wilms, A. Knorr, *Multi-species modeling of quantum dot lasers with microscopic treatment of Coulomb scattering*, in: Proceedings of the 10th International Conference on Numerical Simulation of Optoelectronic Devices, NUSOD 2010, J. Piprek, B. Klein, D. Yoder, eds., IEEE, Piscataway, NJ, USA, 2010, pp. 59–60.

[5] G. Blanchard, N. Krämer, *Kernel partial least squares is universally consistent*, in: Proceedings of the 13th International Conference on Artificial Intelligence and Statistics (AISTATS 2010), Y.W. Teh, M. Titterington, eds., vol. 9 of JMLR Workshop and Conference Proceedings, Journal of Machine Learning Research, Cambridge, MA, USA, 2010, pp. 57–64.

[6] C. Brée, J. Bethge, A. Demircan, E.T. Nibbering, G. Steinmeyer, *On the origin of negative dispersion contributions in filamentary propagation*, in: Conference on Lasers and Electro-Optics (CLEO), OSA Technical Digest (CD), Optical Society of America, 2010, pp. CMU2/1–CMU2/2.

[7] C. Brée, J. Bethge, S. Skupin, L. Bergé, A. Demircan, G. Steinmeyer, *Double self-compression of femtosecond pulses in filaments*, in: Conference on Lasers and Electro-Optics (CLEO), OSA Technical Digest (CD), Optical Society of America, 2010, pp. JThD6/1–JThD6/2.

[8] A. Bradji, J. Fuhrmann, *Some error estimates of the discretization of parabolic equations on general multidimensional nonconforming spatial meshes*, in: Numerical Methods and Applications, I. Dimov, St. Dimova, N. Kolkovska, eds., vol. 6046 of Lecture Notes in Computer Science, Springer, Berlin/Heidelberg, 2010, pp. 369–376.

[9] A. Erdmann, F. Shao, J. Fuhrmann, A. Fiebach, G.P. Patsis, P. Trefonas, *Modeling of double patterning interactions in litho-cure-litho-etch (LCLE) processes*, in: Optical Microlithography XXIII, Part I, M.V. Dusa, W. Conley, eds., vol. 7640 of Proceedings of SPIE, SPIE, 2010, pp. 76400B/1–76400B/12.

[10] J. Fuhrmann, A. Fiebach, G.P. Patsis, *Macroscopic and stochastic modeling approaches to pattern doubling by acid catalyzed cross-linking*, in: Advances in Resist Materials and Processing Technology XXVII, Part I, R.D. Allen, M.H. Somervell, eds., vol. 7639 of Proceedings of SPIE, SPIE, 2010, pp. 76392I/1–76392I/9.

[11] L. Panizzi, A. Fasano, D. Hömberg, *Modeling, analysis and simulations of case hardening of steel*, in: Progress in Industrial Mathematics at ECMI 2008, A. Fitt, J. Norbury, H. Ockendon, E. Wilson, eds., vol. 15 of Mathematics in Industry, Springer, Berlin et al., 2010, pp. 965–970.

[12] D. Hömberg, O. Rott, *Modeling, analysis and stability of milling processes including workpiece effects*, in: Progress in Industrial Mathematics at ECMI 2008, A. Fitt, J. Norbury, H. Ockendon, E. Wilson, eds., vol. 15 of Mathematics in Industry, Springer, Berlin et al., 2010, pp. 493–498.

[13] V. John, M. Roland, *Simulations of 3D/4D precipitation processes in a turbulent flow field*, in: Numerical Mathematics and Advanced Applications 2009, G. Kreiss, P. Lötstedt, A. Målqvist, M. Neytcheva, eds., Springer, Heidelberg et al., 2010, pp. 479– 487.

[14] D. Kern, *Die Welt des Herrn Kuhn*, in: Besser als Mathe — Moderne angewandte Mathematik aus dem MATHEON zum Mitmachen, K. Biermann, M. Grötschel, B. Lutz-Westphal, eds., Reihe: Populär, Vieweg+Teubner, Wiesbaden, 2010, pp. 141–150.

[15] W. König, *Upper tails of self-intersection local times of random walks: Survey of proof techniques*, in: Excess Self-Intersections & Related Topics, vol. 2 of Actes des Rencontres du CIRM, Centre International de Rencontres Mathématiques, Marseille, 2010, pp. 15–24.

[16] A. Jechow, D. Skoczowsky, M. Lichtner, M. Radziunas, R. Menzel, *High-brightness emission from stripe-array broad area diode lasers operated in off-axis external cavities*, in: High-Power Diode Laser Technology and Applications VIII, M.S. Zediker, ed., vol. 7583 of Proceedings of SPIE, SPIE, 2010, pp. 758312/1–758312/11.

[17] A. Mielke, *Existence theory for finite-strain crystal plasticity with gradient regularization*, in: IUTAM Symposium on Variational Concepts with Applications to the Mechanics of Materials, K. Hackl, ed., vol. 21 of IUTAM Bookseries, Springer, Heidelberg, 2010, pp. 171–183.

[18] A. Mielke, L. Paoli, A. Petrov, U. Stefanelli, *Error bounds for space-time discretization of a 3D model for shape-memory materials*, in: IUTAM Symposium on Variational Concepts with Applications to the Mechanics of Materials, K. Hackl, ed., vol. 21 of IUTAM Bookseries, Springer, Heidelberg, 2010, pp. 185–197.

[19] H.-G. Bartel, H.-J. Mucha, J. Dolata, *Geochemical and statistical investigation of Roman stamped tiles of the Legio XXI Rapax*, in: Classification as a Tool for Research. 11th IFCS Biennial Conference and 33rd Annual Conference of the Gesellschaft für Klassifikation e. V., Dresden, March 13–18, 2009, H. Locarek-Junge, C. Weihs, eds., Studies in Classification, Data Analysis, and Knowledge Organization, Springer, Berlin/Heidelberg, 2010, pp. 427–434.

[20] 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, A. Fink, B. Lausen, W. Seidel, A. Ultsch, eds., Studies in Classification, Data Analysis, and Knowledge Organization, Springer, Heidelberg, 2010, pp. 595–603.

[21] ———, *Mathematisch-archäometrische Auswertung der GIS-gestützten Fundkartierung römischer Ziegel aus Mainz*, in: Archäometrie und Denkmalpflege 2010, O. Hahn, A. Hauptmann, D. Modarressi-Tehrani, M. Prange, eds., Metalla, Sonderheft 3, Deutsches Bergbau-Museum Bochum, 2010, pp. 119–121.

[22] J. Dolata, D. Lück, H.-G. Bartel, H.-J. Mucha, C. Wenzel, *Analysen römischer Ziegel aus dem Kastellbad von Groß-Gerau: ihre statistische Auswertung und archäologische Bewertung*, in: Archäometrie und Denkmalpflege 2010, O. Hahn, A. Hauptmann, D. Modarressi-Tehrani, M. Prange, eds., Metalla, Sonderheft 3, Deutsches Bergbau-Museum Bochum, 2010, pp. 129–131.

[23] C. Morales-Merino, H.-J. Mucha, H.-G. Bartel, E. Pernicka, *Clay sediments analysis in the Troad and its segmentation*, in: Archäometrie und Denkmalpflege 2010, O. Hahn, A. Hauptmann, D. Modarressi-Tehrani, M. Prange, eds., Metalla, Sonderheft 3, Deutsches Bergbau-Museum Bochum, 2010, pp. 122–124.

[24] E. Haimerl, H.-J. Mucha, *Comparing the stability of clustering results of dialect data based on several distance matrices*, in: Classification as a Tool for Research. Proceedings of the 11th IFCS Biennial Conference and 33rd Annual Conference of the Gesellschaft für Klassifikation e. V., Dresden, March 13–18, 2009, H. Locarek-Junge, C. Weihs, eds., Studies in Classification, Data Analysis, and Knowledge Organization, Springer, Berlin/Heidelberg, 2010, pp. 665–672.

[25] 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., Reihe: Populär, Vieweg+Teubner, Wiesbaden, 2010, pp. 227–235.

[26] M. Jensen, R. Müller, *Stable Crank–Nicolson discretisation for incompressible miscible displacement problems of low regularity*, in: Numerical Mathematics and Advanced Applications 2009, Part 2, G. Kreiss, P. Lötstedt, A. Målqvist, M. Neytcheva, eds., Springer, Heidelberg et al., pp. 469–477.

[27] P.N. Racec, R. Racec, H. Neidhardt, *R-matrix formalism for electron scattering in two dimensions with applications to nanostructures with quantum dots*, in: Trends in Nanophysics, A. Aldea, V. Bârsan, eds., Engineering Materials, Springer, Berlin/Heidelberg, 2010, pp. 149–174.

[28] M. Radziunas, A.G. Vladimirov, E.A. Viktorov, *Traveling wave modeling, simulation and analysis of quantum-dot mode-locked semiconductor lasers*, in: Semiconductor Lasers and Laser Dynamics IV,

K. Panayotov, M. Sciamanna, A.A. Valle, R. Michalzik, eds., vol. 7720 of Proceedings of SPIE, SPIE, 2010, pp. 77200X/1–77200X/8.

[29] P. Rasper, O. Rott, D. Hömberg, E. Uhlmann, *Analysis of uncertainties in the stability prediction for milling processes*, in: Conference Proceedings, CIRP 2nd International Conference "Process Machine Interactions", June 10–11, 2010, Vancouver (CD), Y. Altintas, B. Denkena, Ch. Brecher, eds., 2010, pp. M18/1–M18/12.

[30] T. Bosse, A. Griewank, L. Lehmann, V. Schlosshauer, *On Hessian- and Jacobian-free SQP methods — A total quasi-Newton scheme with compact storage*, in: Recent Advances in Optimization and its Applications in Engineering, M. Diehl, F. Glineur, E. Jarlebring, W. Michiels, eds., Springer, Berlin/Heidelberg, 2010, pp. 63–72.

[31] G. Schmidt, *Boundary integral methods for periodic scattering problems*, in: Around the Research of Vladimir Maz'ya II. Partial Differential Equations, A. Laptev, ed., vol. 12 of International Mathematical Series, Springer Science+Business Media, New York [et al.], 2010, pp. 337–363.

[32] J.G.M. Schoenmakers, *Optionsbewertung*, in: Besser als Mathe — Moderne angewandte Mathematik aus dem MATHEON zum Mitmachen, K. Biermann, M. Grötschel, B. Lutz-Westphal, eds., Reihe: Populär, Vieweg+Teubner, Wiesbaden, 2010, pp. 187–192.

[33] P. Colli, G. Gilardi, P. Podio-Guidugli, J. Sprekels, *Global solution to a phase transition problem of the Allen–Cahn type*, in: Nonlinear Evolution Equations and Mathematical Modeling, Proceedings of the RIMS Symposium held at the Research Institute for Mathematical Sciences, Kyoto University, October 20–23, 2009, T. Aiki, ed., vol. 1693 of Sūrikaisekikenkyūsho Kōkyūroku, Kyoto, 2010, pp. 104–110.

[34] P. Krejčí, E. Rocca, J. Sprekels, *Liquid-solid phase transitions in a deformable container*, in: Continuous Media with Microstructure, B. Albers, ed., Springer, Berlin/Heidelberg, 2010, pp. 285–300.

[35] K. Tabelow, *Viele Tests — viele Fehler*, in: Besser als Mathe — Moderne angewandte Mathematik aus dem MATHEON zum Mitmachen, K. Biermann, M. Grötschel, B. Lutz-Westphal, eds., Reihe: Populär, Vieweg+Teubner, Wiesbaden, 2010, pp. 117–120.

[36] M. Thomas, *From damage to delamination in nonlinearly elastic materials at small strains*, in: Microstructures in Solids: From Quantum Models to Continua, Workshop, March 14–20, 2010, vol. 7 of Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach, 2010, pp. 783–785.

[37] V.Z. Tronciu, *Semiconductor laser a key element for new generation optoelectronic systems*, in: Proceedings of the 3rd International Conference on Telecommunications, Electronics and Informatics (ICTEI 2010), V. Kantser, S. Andronic, eds., vol. 1, Technical University of Moldova, Chisinau, 2010, pp. 67–72.

[38] I.V. Ermakov, G. Van der Sande, L. Gelens, A. Scire, P. Colet, C.R. Mirasso, V.Z. Tronciu, J. Danckaert, *Numerical investigation of nonlinear dynamics of semiconductor ring lasers with two external cavities*, in: Proceedings of the Young Optical Scientists Conference, YOSC-2009, V. Karassik, ed., Bauman Moscow State Technical University Press, 2010, pp. 106–109.

[39] V.Z. Tronciu, S.S. Rusu, C. Pîrtac, *Dynamics of coupled semiconductor lasers. On/off phase shift keying encryption method*, in: Proceedings of the 3rd International Conference on Telecommunications, Electronics and Informatics (ICTEI 2010), V. Kantser, S. Andronic, eds., vol. 1, Technical University of Moldova, Chisinau, 2010, pp. 77–80.

[40] V.Z. Tronciu, C. Fiebig, M. Lichtner, H. Wenzel, *Numerical and experimental investigations of DBR tapered lasers*, in: Proceedings of the 3rd International Conference on Telecommunications, Electronics and Informatics (ICTEI 2010), V. Kantser, S. Andronic, eds., vol. 1, Technical University of Moldova, Chisinau, 2010, pp. 73–76.

[41] A.G. Vladimirov, M. Wolfrum, G. Fiol, D. Arsenijević, D. Bimberg, E. Viktorov, P. Mandel, D. Rachinskii, *Locking characteristics of a 40-GHz hybrid mode-locked monolithic quantum dot laser*, in: Semiconductor Lasers and Laser Dynamics IV, K. Panajotov, M. Sciamanna, A.A. Valle, R. Michalzik, eds., vol. 7720 of Proceedings of SPIE, SPIE, 2010, pp. 77200Y/1–77200Y/8.

Contributions to Collected Editions (to appear)

[1] C. Guhlke, W. Dreyer, *Hysteresis and phase transition in many-particle storage systems*, in: Proceedings of the 13th International Conference on Hyperbolic Problems: Theory, Numerics, Applications (HYP 2010), Series in Contemporary Applied Mathematics.

[2] R. Henrion, *Probabilistically constrained programming — Models and basic properties*, in: Wiley Encyclopedia of Operations Research and Management Science, J.J. Cochran, ed., Wiley.

[3] N. Dropka, W. Miller, U. Rehse, P. Rudolph, F. Bullesfeld, U. Sahr, O. Klein, D. Reinhardt, *Numerical study on improved mixing in silicon melts by double-frequency TMF*, in: Proceedings of the 16th International Conference on Crystal Growth (ICCG-16), J. Crystal Growth.

[4] W. König, S. Schmidt, *The parabolic Anderson model with acceleration and deceleration*, in: Anniversary publication for Erwin Bolthausen and Jürgen Gärtner, Springer.

[5] M. Lichtner, M. Spreemann, U. Bandelow, *Parallel simulation of high power semiconductor lasers*, in: PARA 2008, 9th International Workshop on State-of-the-Art in Scientific and Parallel Computing, Trondheim, Norway, May 13–16, Lecture Notes in Computer Science, Springer, Berlin/Heidelberg.

[6] R. Haller-Dintelmann, J. Rehberg, *Maximal parabolic regularity for divergence operators on distribution spaces*, in: Nonlinear Parabolic Problems, J. Escher, P. Guidotti, M. Hieber, P. Mucha, J. Pruess, Y. Shibata, G. Simonett, Ch. Walker, eds., Birkhäuser, Basel.

[7] E. Jarlebring, O. Rott, *An iterative method for the multipliers of periodic delay-differential equations and the analysis of a PDE milling model*, in: IFAC Proceedings, Elsevier.

[8] J. Sprekels, *Technical and mathematical problems in the Czochralski growth of single crystals*, in: Mathematics of PDE Constrained Optimization, Seminar, November 21–27, 2010, Oberwolfach Reports, Mathematisches Forschungsinstitut Oberwolfach.

A.6.6 Publications for a More General Public

In the footsteps of Leibniz — The clever people of today

[1] T. Köhler, H. Stephan, G. Wiemer, *Auf Leibniz' Spuren — Die schlauen Leute von heute. Das Weierstraß-Institut für Angewandte Analysis und Stochastik*, Mosaik — Die unglaubliche Reise der Abrafaxe, Steinchen für Steinchen Verlag GmbH, Berlin, no. 413, May 2010, pp. 22–23.

A.7 Preprints, Reports[5]

A.7.1 WIAS Preprints Series

[1] L. Cherkas, A. Grin, K.R. Schneider, *A new approach to study limit cycles on a cylinder*, Preprint no. 1525, WIAS, Berlin, 2010.

[2] K. Fleischmann, L. Mytnik, V. Wachtel, *Properties of states of super- α -stable motion with branching of index $1+\beta$* , Preprint no. 1548, WIAS, Berlin, 2010.

[3] S. Ganesan, *An operator-splitting heterogeneous finite element method for population balance equations: Stability and convergence*, Preprint no. 1531, WIAS, Berlin, 2010.

[4] G.L. Aki, J. Dolbeault, Ch. Sparber, *Thermal effects in gravitational Hartree systems*, Preprint no. 1544, WIAS, Berlin, 2010.

[5] I. Babushkin, W. Kuehn, Ch. Köhler, St. Skupin, L. Bergé, K. Reimann, M. Woerner, J. Herrmann, Th. Elsaesser, *Ultrafast spatio-temporal dynamics of terahertz generation by ionizing two-color femtosecond pulses in gases*, Preprint no. 1488, WIAS, Berlin, 2010.

[6] I. Babushkin, St. Skupin, J. Herrmann, *Generation of terahertz radiation from ionizing two-color laser pulses in Ar filled metallic hollow waveguides*, Preprint no. 1483, WIAS, Berlin, 2010.

[7] I. Babushkin, U. Bandelow, A. Vladimirov, *Rotational symmetry breaking in small-area circular vertical cavity surface emitting lasers*, Preprint no. 1526, WIAS, Berlin, 2010.

[8] M. Becker, W. König, *Self-intersection local times of random walks: Exponential moments in subcritical dimensions*, Preprint no. 1532, WIAS, Berlin, 2010.

[9] S. Becker, *Regularization of statistical inverse problems and the Bakushinskii veto*, Preprint no. 1564, WIAS, Berlin, 2010.

[10] D. Belomestny, *On the rates of convergence of simulation-based optimization algorithms for optimal stopping problems*, Preprint no. 1495, WIAS, Berlin, 2010.

[11] ———, *Pricing Bermudan options using regression: Optimal rates of convergence for lower estimates*, Preprint no. 1492, WIAS, Berlin, 2010.

[12] ———, *Spectral estimation of the fractional order of a Lévy process*, Preprint no. 1491, WIAS, Berlin, 2010.

[13] D. Belomestny, V. Krätschmer, *Central limit theorems for law-invariant coherent risk measures*, Preprint no. 1551, WIAS, Berlin, 2010.

[14] C. Brée, J. Bethge, St. Skupin, L. Bergé, A. Demircan, G. Steinmeyer, *Cascaded self-compression of femtosecond pulses in filaments*, Preprint no. 1478, WIAS, Berlin, 2010.

[15] J. Bethge, G. Steinmeyer, G. Stibenz, P. Staudt, C. Brée, A. Demircan, H. Redlin, St. Düsterer, *Self-compression of 120 fs pulses in a white-light filament*, Preprint no. 1529, WIAS, Berlin, 2010.

[16] C. Brée, A. Demircan, G. Steinmeyer, *Modulation instability in filamentary self-compression*, Preprint no. 1570, WIAS, Berlin, 2010.

[17] C. Brée, A. Demircan, G. Steinmeyer, *Saturation of the all-optical Kerr effect*, Preprint no. 1540, WIAS, Berlin, 2010.

[18] W. Dreyer, C. Guhlke, M. Herrmann, *Hysteresis and phase transition in many-particle storage systems*, Preprint no. 1481, WIAS, Berlin, 2010.

[5] Preprints and reports 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] W. Dreyer, J. Giesselmann, Ch. Kraus, Ch. Rohde, *Asymptotic analysis for Korteweg models*, Preprint no. 1545, WIAS, Berlin, 2010.

[20] P.-E. Druet, *The classical solvability of the contact angle problem for generalized equations of mean curvature type*, Preprint no. 1576, WIAS, Berlin, 2010.

[21] P.-É. Druet, *Global Lipschitz continuity for elliptic transmission problems with a boundary intersecting interface*, Preprint no. 1571, WIAS, Berlin, 2010.

[22] P.-É. Druet, P. Philip, *Noncompactness of integral operators modeling diffuse-gray radiation in polyhedral and transient settings*, Preprint no. 1493, WIAS, Berlin, 2010.

[23] J. Ehrt, *Parameterizations of sub-attractors in hyperbolic balance laws*, Preprint no. 1518, WIAS, Berlin, 2010.

[24] J. Elschner, G. Hu, *Global uniqueness in determining polygonal periodic structures with a minimal number of incident plane waves*, Preprint no. 1498, WIAS, Berlin, 2010.

[25] ———, *Inverse scattering of elastic waves by periodic structures: Uniqueness under the third or fourth kind boundary conditions*, Preprint no. 1528, WIAS, Berlin, 2010.

[26] ———, *Inverse scattering of electromagnetic waves by multilayered structures: Uniqueness in TM mode*, Preprint no. 1549, WIAS, Berlin, 2010.

[27] ———, *Scattering of plane elastic waves by three-dimensional diffraction gratings*, Preprint no. 1565, WIAS, Berlin, 2010.

[28] J. Elschner, G.C. Hsiao, A. Rathsfeld, *Comparison of numerical methods for the reconstruction of elastic obstacles from the far-field data of scattered acoustic waves*, Preprint no. 1479, WIAS, Berlin, 2010.

[29] Ch. Batallion, F. Bouchon, C. Chainais-Hillairet, J. Fuhrmann, E. Hoarau, R. Touzani, *Numerical methods for the simulation of a corrosion model in a nuclear waste deep repository*, Preprint no. 1575, WIAS, Berlin, 2010.

[30] J. Fuhrmann, H. Langmach, A. Linke, *A numerical method for mass conservative coupling between fluid flow and solute transport*, Preprint no. 1521, WIAS, Berlin, 2010.

[31] J. Fuhrmann, H. Zhao, H. Langmach, Y.E. Seidel, Z. Jusys, R.J. Behm, *The role of reactive reaction intermediates in two-step heterogeneous electro-catalytic reactions: A model study*, Preprint no. 1522, WIAS, Berlin, 2010.

[32] A. Glitzky, *Analysis of electronic models for solar cells including energy resolved defect densities*, Preprint no. 1524, WIAS, Berlin, 2010.

[33] Ch. Heinemann, Ch. Kraus, *Existence of weak solutions for Cahn–Hilliard systems coupled with elasticity and damage*, Preprint no. 1520, WIAS, Berlin, 2010.

[34] Ch. Heinemann, Ch. Kraus, *Existence results for diffuse interface models describing phase separation and damage*, Preprint no. 1569, WIAS, Berlin, 2010.

[35] M.J. Fabian, R. Henrion, A.Y. Kruger, J. Outrata, *Error bounds: Necessary and sufficient conditions*, Preprint no. 1477, WIAS, Berlin, 2010.

[36] R. Henrion, A. Seeger, *Inradius and circumradius of various convex cones arising in applications*, Preprint no. 1505, WIAS, Berlin, 2010.

[37] ———, *On properties of different notions of centers for convex cones*, Preprint no. 1476, WIAS, Berlin, 2010.

[38] R. Henrion, Th. Surowiec, *On calmness conditions in convex bilevel programming*, Preprint no. 1508, WIAS, Berlin, 2010.

[39] D. Hömberg, E. Rocca, *A model for resistance welding including phase transitions and Joule heating*, Preprint no. 1496, WIAS, Berlin, 2010.

[40] R. Haller-Dintelmann, W. Höppner, H.-Chr. Kaiser, J. Rehberg, G. Ziegler, *Optimal elliptic Sobolev regularity near three-dimensional, multi-material Neumann vertices*, Preprint no. 1515, WIAS, Berlin, 2010.

[41] G. Hu, J. Yang, B. Zhang, *An inverse electromagnetic scattering problem for a bi-periodic inhomogeneous layer on a perfectly conducting plate*, Preprint no. 1499, WIAS, Berlin, 2010.

[42] M. Aizenman, S. Jansen, P. Jung, *Symmetry breaking in quasi-1D Coulomb systems*, Preprint no. 1547, WIAS, Berlin, 2010.

[43] V. John, J. Novo, *Error analysis of the SUPG finite element discretization of evolutionary convection-diffusion-reaction equations*, Preprint no. 1494, WIAS, Berlin, 2010.

[44] V. John, P. Knobloch, S.B. Savescu, *A posteriori optimization of parameters in stabilized methods for convection-diffusion problems — Part I*, Preprint no. 1527, WIAS, Berlin, 2010.

[45] H.-Chr. Kaiser, J. Rehberg, *Optimal elliptic regularity at the crossing of a material interface and a Neumann boundary edge*, Preprint no. 1511, WIAS, Berlin, 2010.

[46] N. Kleemann, *Shape derivatives in Kondratiev spaces for conical diffraction*, Preprint no. 1489, WIAS, Berlin, 2010.

[47] W. König, *Upper tails of self-intersection local times of random walks: Survey of proof techniques*, Preprint no. 1568, WIAS, Berlin, 2010.

[48] W. König, P. Schmid, *Brownian motion in a truncated Weyl chamber*, Preprint no. 1533, WIAS, Berlin, 2010.

[49] W. König, S. Schmidt, *The parabolic Anderson model with acceleration and deceleration*, Preprint no. 1552, WIAS, Berlin, 2010.

[50] St. Adams, A. Collevecchio, W. König, *A variational formula for the free energy of an interacting many-particle system*, Preprint no. 1490, WIAS, Berlin, 2010.

[51] Th. Koprucki, A. Wilms, A. Knorr, U. Bandelow, *Modeling of quantum dot lasers with microscopic treatment of Coulomb effects*, Preprint no. 1543, WIAS, Berlin, 2010.

[52] M.D. Korzec, P. Nayar, P. Rybka, *Global weak solutions to a sixth order Cahn–Hilliard type equation*, Preprint no. 1581, WIAS, Berlin, 2010.

[53] M.D. Korzec, P. Rybka, *On a higher order convective Cahn–Hilliard type equation*, Preprint no. 1582, WIAS, Berlin, 2010.

[54] T. Krueger, N. Krämer, K. Rieck, *ASAP: Automatic semantics-aware analysis of network payloads*, Preprint no. 1502, WIAS, Berlin, 2010.

[55] N. Krämer, M. Sugiyama, *The degrees of freedom of partial least squares regression*, Preprint no. 1487, WIAS, Berlin, 2010.

[56] V. Krätschmer, H. Zähle, *Sensitivity of risk measures with respect to the normal approximation of total claim distributions*, Preprint no. 1519, WIAS, Berlin, 2010.

[57] Ch. Kraus, *The degenerate and non-degenerate Stefan problem with inhomogeneous and anisotropic Gibbs–Thomson law*, Preprint no. 1567, WIAS, Berlin, 2010.

[58] K. Krumbiegel, I. Neitzel, A. Rösch, *Regularization error estimates for semilinear elliptic optimal control problems with pointwise state and control constraints*, Preprint no. 1480, WIAS, Berlin, 2010.

[59] ———, *Sufficient optimality conditions for the Moreau–Yosida-type regularization concept applied to semilinear elliptic optimal control problems with pointwise state constraints*, Preprint no. 1503, WIAS, Berlin, 2010.

[60] M. Liero, A. Mielke, *An evolutionary elastoplastic plate model derived via Gamma-convergence*, Preprint no. 1583, WIAS, Berlin, 2010.

[61] A.L. Bowers, B.R. Cousins, A. Linke, L.G. Rebholz, *New connections between finite element formulations of the Navier–Stokes equations*, Preprint no. 1516, WIAS, Berlin, 2010.

[62] M. Case, V. Ervin, A. Linke, L. Rebholz, *Improving mass conservation in FE approximations of the Navier Stokes equations using continuous velocity fields: A connection between grad-div stabilization and Scott–Vogelius elements*, Preprint no. 1510, WIAS, Berlin, 2010.

[63] M. Case, V. Ervin, A. Linke, L. Rebholz, N. Wilson, *Stable computing with an enhanced physics based scheme for the 3D Navier–Stokes equations*, Preprint no. 1509, WIAS, Berlin, 2010.

[64] R. Eymard, Th. Gallouët, R. Herbin, A. Linke, *Convergence of a finite volume scheme for the biharmonic problem*, Preprint no. 1482, WIAS, Berlin, 2010.

[65] J. Flemming, B. Hofmann, P. Mathé, *Sharp converse results for the regularization error using distance functions*, Preprint no. 1535, WIAS, Berlin, 2010.

[66] W. Kirsch, B. Metzger, P. Müller, *Random block operators*, Preprint no. 1538, WIAS, Berlin, 2010.

[67] A. Mielke, *Formulation of thermo-elastic dissipative material behavior using GENERIC*, Preprint no. 1486, WIAS, Berlin, 2010.

[68] ———, *A gradient structure for reaction-diffusion systems and for energy-drift-diffusion systems*, Preprint no. 1485, WIAS, Berlin, 2010.

[69] S. Bartels, A. Mielke, T. Roubíček, *Quasistatic small-strain plasticity in the limit of vanishing hardening and its numerical approximation*, Preprint no. 1585, WIAS, Berlin, 2010.

[70] A. Mielke, L. Truskinovsky, *From discrete visco-elasticity to continuum rate-independent plasticity: Rigorous results*, Preprint no. 1541, WIAS, Berlin, 2010.

[71] A. Mielke, S. Zelik, *On the vanishing-viscosity limit in parabolic systems with rate-independent dissipation terms*, Preprint no. 1500, WIAS, Berlin, 2010.

[72] A. Mielke, T. Roubíček, M. Thomas, *From damage to delamination in nonlinearly elastic materials at small strains*, Preprint no. 1542, WIAS, Berlin, 2010.

[73] S. Bartels, R. Müller, *Error control for the approximation of Allen–Cahn and Cahn–Hilliard equations with a logarithmic potential*, Preprint no. 1539, WIAS, Berlin, 2010.

[74] V.A. Panov, *Estimation of the signal subspace without estimation of the inverse covariance matrix*, Preprint no. 1546, WIAS, Berlin, 2010.

[75] ———, *Non-Gaussian component analysis: New ideas, new proofs, new applications*, Preprint no. 1501, WIAS, Berlin, 2010.

[76] K. Kostourou, D. Peschka, A. Münch, B. Wagner, St. Herminghaus, R. Seemann, *Interface morphologies in liquid/liquid dewetting*, Preprint no. 1560, WIAS, Berlin, 2010.

[77] A. Petrov, *On the numerical approximation of a viscoelastodynamic problem with unilateral constraints*, Preprint no. 1523, WIAS, Berlin, 2010.

[78] J. Polzehl, K. Tabelow, *Beyond the diffusion tensor model: The package dti*, Preprint no. 1563, WIAS, Berlin, 2010.

[79] J. Polzehl, H.U. Voss, K. Tabelow, *Structural adaptive segmentation for statistical parametric mapping*, Preprint no. 1484, WIAS, Berlin, 2010.

[80] R. Racec, U. Wulf, P.N. Racec, *Fano regime of transport through open quantum dots*, Preprint no. 1504, WIAS, Berlin, 2010.

[81] M. Radziunas, K.-H. Hasler, B. Sumpf, T.Q. Tien, H. Wenzel, *Mode transitions in DBR semiconductor lasers: Experiments, mode analysis and simulations*, Preprint no. 1513, WIAS, Berlin, 2010.

[82] M. Radziunas, A.G. Vladimirov, E.A. Viktorov, *Traveling wave modeling, simulation and analysis of quantum-dot mode-locked semiconductor lasers*, Preprint no. 1506, WIAS, Berlin, 2010.

[83] M. Radziunas, A.G. Vladimirov, E.A. Viktorov, G. Fiol, H. Schmeckebier, D. Bimberg, *Broadening of mode-locking pulses in quantum-dot semiconductor lasers: Simulation, analysis and experiments*, Preprint no. 1584, WIAS, Berlin, 2010.

[84] ———, *Strong asymmetry of mode-locking pulses in quantum-dot semiconductor lasers*, Preprint no. 1579, WIAS, Berlin, 2010.

[85] S.B. Savescu, *A substitute for the maximum principle for singularly perturbed time-dependent semilinear reaction-diffusion problems — Part I*, Preprint no. 1550, WIAS, Berlin, 2010.

[86] S.B. Savescu, *A substitute for the maximum principle for singularly perturbed time-dependent semilinear reaction-diffusion problems II. Upper and lower solutions for problems with Neumann boundary conditions*, Preprint no. 1566, WIAS, Berlin, 2010.

[87] J.G.M. Schoenmakers, J. Huang, *Optimal dual martingales and their stability; fast evaluation of Bermudan products via dual backward regression*, Preprint no. 1574, WIAS, Berlin, 2010.

[88] A. Mahayni, J.G.M. Schoenmakers, *Minimum return guarantees with funds switching rights — An optimal stopping problem*, Preprint no. 1534, WIAS, Berlin, 2010.

[89] H. Si, K. Gärtner, *3D boundary recovery by constrained Delaunay tetrahedralization*, Preprint no. 1530, WIAS, Berlin, 2010.

[90] J. Sprekels, D. Tiba, *Extensions of the control variational method*, Preprint no. 1572, WIAS, Berlin, 2010.

[91] P. Colli, P. Krejčí, E. Rocca, J. Sprekels, *A nonlocal quasilinear multi-phase system with nonconstant specific heat and heat conductivity*, Preprint no. 1580, WIAS, Berlin, 2010.

[92] T. Streckenbach, *Parameter determination of an evolution model for phase transformations in steel*, Preprint no. 1512, WIAS, Berlin, 2010.

[93] K. Tabelow, J. Polzehl, *Statistical parametric maps for functional MRI experiments in R: The package fmri*, Preprint no. 1562, WIAS, Berlin, 2010.

[94] K. Tabelow, J.D. Clayden, P. Lafayede Micheaux, J. Polzehl, V.J. Schmid, B. Whitcher, *Image analysis and statistical inference in neuroimaging with R*, Preprint no. 1578, WIAS, Berlin, 2010.

[95] K. Tabelow, H.U. Voss, J. Polzehl, *Modeling the orientation distribution function by mixtures of angular central Gaussian distributions*, Preprint no. 1559, WIAS, Berlin, 2010.

[96] P. Suwanpinij, N. Togobytska, U. Prahl, W. Weiss, D. Hömberg, W. Bleck, *Numerical cooling strategy design for hot rolled dual phase steel*, Preprint no. 1507, WIAS, Berlin, 2010.

[97] A.G. Vladimirov, R. Lefever, M. Tlidi, *Relative stability of multipeak localized patterns*, Preprint no. 1514, WIAS, Berlin, 2010.

[98] A.G. Vladimirov, U. Bandelow, G. Fiol, D. Arsenijević, M. Kleinert, D. Bimberg, A. Pimenov, D. Rachinskii, *Dynamical regimes in a monolithic passively mode-locked quantum dot laser*, Preprint no. 1517, WIAS, Berlin, 2010.

[99] N. Rebrova, G. Huyet, D. Rachinskii, A.G. Vladimirov, *An optically injected mode locked laser*, Preprint no. 1561, WIAS, Berlin, 2010.

[100] M. Grote, V. Palumberi, B. Wagner, A. Barbero, I. Martin, *Dynamic formation of oriented patches in chondrocyte cell cultures*, Preprint no. 1557, WIAS, Berlin, 2010.

[101] G. Kitavtsev, L. Recke, B. Wagner, *Asymptotics for the spectrum of a thin film equation in a singular limit*, Preprint no. 1555, WIAS, Berlin, 2010.

[102] ———, *Center manifold reduction approach for the lubrication equation*, Preprint no. 1554, WIAS, Berlin, 2010.

[103] A. Münch, B. Wagner, *Impact of slippage on the morphology and stability of a dewetting rim*, Preprint no. 1556, WIAS, Berlin, 2010.

[104] A. Münch, C.P. Please, B. Wagner, *Spin coating of an evaporating polymer solution*, Preprint no. 1558, WIAS, Berlin, 2010.

[105] W. Wagner, *Stochastic models in kinetic theory*, Preprint no. 1536, WIAS, Berlin, 2010.

[106] O. Muscato, W. Wagner, V. Di Stefano, *Properties of the steady state distribution of electrons in semiconductors*, Preprint no. 1537, WIAS, Berlin, 2010.

[107] O. Kastner, G.J. Ackland, G. Eggeler, W. Weiss, *A molecular dynamics view of hysteresis and functional fatigue in martensitic transformations*, Preprint no. 1497, WIAS, Berlin, 2010.

[108] A. Schnitzler, T. Wolff, *Precise asymptotics for the parabolic Anderson model with a moving catalyst or trap*, Preprint no. 1553, WIAS, Berlin, 2010.

[109] B. Fiedler, C. Rocha, M. Wolfrum, *A permutation characterization of Sturm attractors of Hamiltonian type*, Preprint no. 1573, WIAS, Berlin, 2010.

[110] M. Wolfrum, O. Omel'chenko, S. Yanchuk, Y. Maistrenko, *Spectral properties of chimera states*, Preprint no. 1577, WIAS, Berlin, 2010.

A.7.2 WIAS Reports Series

[1] J. Ehrt, *Cascades of heteroclinic connections in hyperbolic balance laws*, WIAS Report no. 27, WIAS, Berlin, 2010.

[2] J. Fuhrmann, *Modellierung, experimentelle Untersuchung und Simulation für Direkt-Methanol-Mikrobrennstoffzellen (MikroDMFC)*, WIAS Report no. 28, WIAS, Berlin, 2010.

A.7.3 WIAS Technical Reports Series

[1] T. Streckenbach, *WPM package manager version 1.0 — Software documentation*, WIAS Technical Report no. 12, WIAS, Berlin, 2010.

A.7.4 Preprints/Reports in other Institutions

[1] M. Beiglboeck, P. Friz, St. Sturm, *Is the minimum value of an option on variance generated by local volatility?*, arXiv:1001.4031, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[2] J. Diehl, P. Friz, *Backward stochastic differential equations with rough drivers*, arXiv:1008.0290, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[3] P. Friz, S. Gerhold, A. Gulisashvili, St. Sturm, *On refined volatility smile expansion in the Heston model*, arXiv:1001.3003, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[4] P. Friz, H. Oberhauser, *A generalized Fernique theorem and applications*, arXiv:1004.1923, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[5] ———, *On the splitting-up method for rough (partial) differential equations*, arXiv:1008.0513, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[6] ———, *Rough path stability of SPDEs arising in non-linear filtering*, arXiv:1005.1781, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[7] J. Becker, K. Gärtner, R. Klanner, R. Richter, *Simulation and experimental study of plasma effects in planar silicon sensors*, arXiv:1007.4433, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[8] W. van Ackooij, R. Henrion, A. Möller, R. Zorgati, *On joint probabilistic constraints with Gaussian coefficient matrix*, Preprint no. 6, Stochastic Programming E-Print Series (SPEPS), Humboldt-Universität zu Berlin, 2010.

[9] G. Hu, B. Zhang, *The linear sampling method for the inverse electromagnetic scattering by a partially coated bi-periodic structure*, arXiv:1003.3067, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[10] J. Kampen, *Characteristic functions of affine processes via calculus of their operator symbols*, arXiv:1002.2764, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[11] Ch. Fries, J. Kampen, *On a class of semi-elliptic diffusion models. Part I: A constructive analytical approach for global existence, densities, and numerical schemes with applications to the Libor market model*, arXiv:1002.5031, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[12] A. Fiaschi, D. Knees, U. Stefanelli, *Young measure quasi-static damage evolution*, Preprint no. 28PV10/26/0, Istituto di Matematica Applicata e Technologie Informatiche, Pavia, Italy, 2010.

[13] A. Kyprianou, R.L. Loeffen, J.-L. Perez, *Optimal control with absolutely continuous strategies for spectrally negative Levy processes*, arXiv:1008.2363, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[14] R.L. Loeffen, P. Patie, *Absolute ruin in the Ornstein–Uhlenbeck type risk model*, arXiv:1006.2712, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[15] Ch. Bayer, P. Friz, R.L. Loeffen, *Semi-closed form cubature and applications to financial diffusion models*, arXiv:1009.4818, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[16] A. Mielke, *On an evolutionary model for complete damage based on energies and stresses*, Preprint no. 29PV10/27/0, pp. 23–32, in: Rate-independent evolutions and material modeling, T. Roubíček, U. Stefanelli (eds.), Istituto di Matematica Applicata e Technologie Informatiche, Pavia, Italy, 2010.

[17] A. Mielke, R. Rossi, G. Savaré, *A vanishing viscosity approach to rate-independent modelling in metric spaces*, Preprint no. 29PV10/27/0, pp. 33–38, in: Rate-independent evolutions and material modeling, T. Roubíček, U. Stefanelli (eds.), Istituto di Matematica Applicata e Technologie Informatiche, Pavia, Italy, 2010.

[18] N. Serdyukova, *Local parametric estimation under noise misspecification in regression*, arXiv:0912.4489, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[19] P. Colli, G. Gilardi, P. Podio-Guidugli, J. Sprekels, *A temperature-dependent phase segregation problem of the Allen–Cahn type*, arXiv:1005.0911, Cornell University Library, arXiv.org, Ithaca, USA, 2010.

[20] A. Braumann, M. Kraft, W. Wagner, *Numerical study of a stochastic particle algorithm solving a multidimensional population balance model for high shear granulation*, Technical Report no. 93, c4e-Preprint Series, Cambridge Centre for Computational Chemical Engineering, University of Cambridge, Department of Chemical Engineering, UK, 2010.

A.8 Talks, Posters, and Contributions to Exhibitions[6]

A.8.1 Main Talks

1. R. Henrion, *Optimization problems with probabilistic constraints*, 3rd International Conference on Continuous Optimization (ICCOPT), July 26–29, Santiago de Chile, July 27.
2. ———, *Chance-constrained problems*, Pre-Conference PhD Workshop, 12th Conference on Stochastic Programming (SPXII), Halifax, Canada, August 15.
3. J. Sprekels, *Mathematical problems in industrial crystal growth: Radiation, magnetic fields, and free boundaries*, Symposium zur Angewandten Mathematik (zum 100. Geburtstag von Lothar Collatz), October 7–8, Universität Hamburg, October 7.

A.8.2 Scientific Talks (Invited)

1. P. Friz, *Stochastic analysis and quantitative finance*, Microsoft Research Cambridge, UK, January 5.
2. ———, *Applications of rough path theory to stochastic analysis*, Workshop "Rough Paths in Interaction", June 10–11, Université Pierre et Marie Curie (UPMC), Institut Henri Poincaré, Paris, France, June 10.
3. ———, *Rough path stability of SPDEs arising in non-linear filtering and beyond*, Workshop on Filtering, June 14–15, University of Cambridge, Isaac Newton Institute for Mathematical Sciences, UK, June 15.
4. ———, *Rough viscosity solutions and applications to SPDEs*, Workshop on Stochastic Partial Differential Equations (SPDEs): Approximation, Asymptotics and Computation, June 28 – July 2, University of Cambridge, Isaac Newton Institute for Mathematical Sciences, UK, June 29.
5. ———, *Ordinary, partial and backward stochastic differential equations driven by rough signals*, Analysis, Stochastics, and Applications (AnStAp 2010), July 12–16, Universität Wien, Fakultät für Mathematik, Austria, July 13.
6. ———, *A (rough) pathwise approach to SPDEs*, ICM Satellite Conference on Probability and Stochastic Processes, August 13–17, Indian Statistical Institute, Bangalore, India, August 16.
7. ———, *A new pathwise theory of SPDEs*, 34th Conference on Stochastic Processes and their Applications (SPA 2010), September 6–10, Bernoulli Society for Mathematical Statistics and Probability, Osaka, Japan, September 9.
8. ———, *Ordinary, partial and backward stochastic differential equations driven by rough paths*, Conference in Memory of Paul Malliavin, October 4–6, Institut de Mathématiques de Bourgogne, Dijon, France, October 6.
9. S. Amiranashvili, *Propagation of ultrashort optical pulses*, Matheon Workshop "4th Annual Meeting Photonic Devices", Zuse Institute Berlin, February 18.
10. U. Bandelow, *Semiconductor laser instabilities and dynamics (short course)*, 10th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD) 2010, September 6–9, Atlanta, USA, September 6.
11. ———, *Dynamics in semiconductor lasers and propagation of ultrashort pulses in nonlinear fibers*, Institut für Photonische Technologien, Arbeitsgruppe Laserdiagnostik, Jena, September 30.

[6] Contributions by scholarship holders and guests during their stay at WIAS have been listed in front of those made by the collaborators of WIAS.

12. ———, *Semiconductor lasers for high speed applications: Modeling and simulation*, International Workshop on High Speed Semiconductor Lasers (HSSL 2010), October 7–8, Wroclaw University of Technology, Institute of Physics, Poland, October 7.

13. D. Belomestny, *Modern methods of option pricing*, Postbank Bonn, February 25.

14. ———, *Estimating the distribution of jumps in regular affine models: Uniform rates of convergence*, Leipziger Stochastik-Tage, March 1–5, Universität Leipzig, Fakultät für Mathematik und Informatik, March 2.

15. ———, *On the rates of convergence of simulation-based optimization algorithms for optimal stopping problems*, Leipziger Stochastik-Tage, March 1–5, Universität Leipzig, Fakultät für Mathematik und Informatik, March 3.

16. ———, *Statistical inference for multidimensional time-changed Levy processes based on low-frequency data*, Universität Bayreuth, Fachbereich Mathematik, July 27.

17. G. Blanchard, *On optimal rates for kernel conjugate gradient regularization under random design and noise*, Mini Special Semester on Inverse Problems, Part II: "Inverse Problems in Data Driven Modelling", July 19–22, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, July 20.

18. A. Caiazzo, *Blood flow through a porous interface: Numerical schemes and applications*, IV International Symposium on Modeling of Physiological Flows 2010 (MPF2010), June 2–5, Cagliari, Italy, June 5.

19. E. Diederichs, *Semidefinite non-Gaussian component analysis*, Project Workshop "PAKT: Multiple Testing", Deutsches Diabetes Zentrum Düsseldorf, June 17.

20. W. Dreyer, *Hysteresis and phase transition in many-particle electrodes for lithium-ion batteries*, 24th Annual MSIT Meeting — International Seminar on Heterogeneous Multicomponent Equilibria, Schloss Ringberg, Kreuth, February 12.

21. ———, *Modeling and simulations of storage problems for rechargeable lithium-ion batteries*, Colloquium of the DFG Priority Program SPP 1473 "WeNDeLIB", March 16–18, Tagungszentrum Deutsches Brennstoffinstitut, Freiberg, March 17.

22. ———, *Modeling of non-isothermal liquid-vapor transitions*, 5th Workshop "Micro-Macro Modelling and Simulation of Liquid-Vapour Flows", April 14–16, Strasbourg, France, April 15.

23. ———, *On a paradox within the phase field modeling of storage systems and its resolution*, 8th AIMS International Conference on Dynamical Systems, Differential Equations and Applications, May 25–28, Technische Universität Dresden, May 26.

24. ———, *Hysteresis of many-particle systems due to non-monotone constitutive behavior*, Workshop "Phase Transitions", May 31 – June 4, Mathematisches Forschungsinstitut Oberwolfach, May 31.

25. ———, *Hysteresis and phase transition in many-particle storage systems*, 13th International Conference on Hyperbolic Problems: Theory, Numerics, Applications (HYP 2010), June 14–19, Beijing, China, June 17.

26. ———, *Modelling and simulations of a scalar conservation law in the context of Lithium-ion batteries and a system of interconnected air balloons*, Kolloquium Prof. Freistühler, Universität Konstanz, July 6.

27. ———, *Pieces of thermodynamics of fluidic interfaces*, Summer School of the DFG Priority Program 1506 "Transport Processes at Fluidic Interfaces", Technische Universität Darmstadt, Center of Smart Interfaces, July 8.

28. ———, *Hysteresis and phase transitions in many-particle storage systems*, XVII International ISIMM Conference on Trends in Applications of Mathematics to Mechanics (STAMM 2010), August 30 – September 2, Schmöckwitz, August 30.

29. ———, *The effect of entropy of mixing on phase transitions*, DFG-CNRS Workshop on Phase Field Models, September 27–30, Freiburg, September 29.

30. J. Ehrt, *Cascades of heteroclinic connections in viscous balance laws*, 8th AIMS International Conference on Dynamical Systems, Differential Equations and Applications, May 25–28, Technische Universität Dresden, May 27.

31. J. Elschner, *On uniqueness in inverse elastic obstacle scattering*, University of Tokyo, Department of Mathematical Sciences, Japan, March 23.

32. J. Fuhrmann, *Aspects of numerical simulation of semiconductor photoresists*, Université Blaise Pascal, Clermont-Ferrand II, France, June 10.

33. T. Girnyk, *Multistability of twisted states in non-locally coupled Kuramoto-type models*, Universität Potsdam, Institut für Physik und Astronomie, October 25.

34. ———, *Multistability of twisted states in non-locally coupled Kuramoto-type models*, École Polytechnique Fédérale de Lausanne, Laboratory of Nonlinear Systems (EPFL-LANOS), Switzerland, November 17.

35. A. Glitzky, *Uniform exponential decay of the free energy for Voronoi finite volume discretized reaction-diffusion systems*, 8th AIMS International Conference on Dynamical Systems, Differential Equations and Applications, Special Session on Reaction Diffusion Systems, May 25–28, Technische Universität Dresden, May 26.

36. C. Guhlke, *Hysteresis and phase transition in many-particle electrodes for lithium-ion batteries*, 24th Annual MSIT Meeting — International Seminar on Heterogeneous Multicomponent Equilibria, Schloss Ringberg, Kreuth, February 12.

37. ———, *Hysteresis due to non-monotone material behaviour inside many-particle systems*, DPG Spring Meeting 2010, March 21–26, Regensburg, March 25.

38. ———, *Hysteresis due to non-monotone material behaviour inside many-particle systems*, SIAM Conference on Mathematical Aspects of Materials Science (MS10), May 23–26, Philadelphia, USA, May 23.

39. D. Hömberg, *The mathematics of distortion*, "Seminario Matematico e Fisico di Milano", Università di Milano, Dipartimento di Matematica, Italy, March 1.

40. ———, *A brief introduction to PDE-constrained control*, Warsaw Seminar on Industrial Mathematics (WSIM'10), March 18–19, Warsaw University of Technology, Poland, March 18.

41. ———, *Coupling of process, machine, and work-piece in production processes — A challenge for industrial mathematics*, Warsaw Seminar on Industrial Mathematics (WSIM'10), March 18–19, Warsaw University of Technology, Poland, March 19.

42. ———, *Steel manufacturing — A challenge for applied mathematics*, Universität Duisburg-Essen, Fachbereich Mathematik, May 11.

43. ———, *On a thermomechanical milling model*, Workshop "Rate-independent Systems: Modeling, Analysis, and Computations", August 30 – September 3, Banff International Research Station for Mathematical Innovation and Discovery (BIRS), Canada, August 31.

44. ———, *Modelling, simulation and control of phase transformations in steel*, Nippon Steel Corporation, Chiba, Japan, September 10.

45. ———, *Multiphase steels, heat treatment and distortion — Mathematical challenges in steel production and manufacturing*, Summer School "High Performance Computing" (organizer: TU Ilmenau), September 29 – October 2, Upstalsboom Hotel Friedrichshain, Berlin, September 30.

46. ———, *Manufacturing and processing of steel — A challenge for industrial mathematics*, Forum "Math for Industry" 2010, October 21–23, Fukuoka, Japan, October 21.

47. G. Hu, *Variational approach to scattering of elastic waves by doubly periodic structures*, Chinese Academy of Sciences, LSEC and Institute of Applied Mathematics, Beijing, Republic of China, May 6.

48. ———, *Uniqueness in inverse wave scattering by unbounded obstacles*, The Fifth International Conference on Inverse Problems, December 13–17, City University of Hong Kong, Republic of China, December 15.

49. ———, *Scattering of electromagnetic waves by three-dimensional diffraction gratings*, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Institute of Applied Mathematics, Beijing, Republic of China, December 22.

50. V. John, *Finite element methods for the simulation of incompressible turbulent flows*, 6 talks, Deutsch-Französische Sommerschule "Modellierung, numerische Simulation und Optimierung in der Strömungsmechanik", September 6–10, Karlsruher Institut für Technologie, Bad Herrenalb.

51. ———, *Incompressible flow simulations with finite element methods*, 4 talks, February 22–26, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain.

52. ———, *A posteriori optimization of parameters in stabilized methods for convection-diffusion problems*, BIRS Workshop "Nonstandard Discretizations for Fluid Flows", November 21–26, Banff International Research Station, Canada.

53. ———, *On the numerical simulation of population balance systems*, Technische Universität Dresden, Fakultät Mathematik und Naturwissenschaften, April 20.

54. ———, *Error analysis of the SUPG finite element discretization of evolutionary convection-diffusion-reaction equations*, 6th Variational Multiscale Methods Workshop (VMS 2010), May 27–28, Université de Pau et des Pays de l'Adour, France, May 27.

55. ———, *Variational multiscale methods for the simulation of turbulent flows*, Volkswagen Wolfsburg, August 27.

56. ———, *On the analysis and numerical analysis of turbulence models*, Workshop on Calibration of Viscosity Models for Turbulent Flows, October 8–9, Georg-August-University Göttingen, October 8.

57. ———, *Numerical methods for the simulation of population balance systems*, Symposium on Analysis and Control of Infinite-Dimensional Systems in the Engineering Sciences (ACIDS), November 18–19, Max-Planck-Institut für Dynamik komplexer technischer Systeme, Magdeburg, November 19.

58. J. Kampen, *On a class of semi-elliptic diffusion models. Part I: A constructive analytical approach for global existence, densities, and numerical schemes (with applications to the Libor market model)*, Postbank Bonn, February 25.

59. ———, *On a class of semi-elliptic diffusion models*, Mathematisches Kolloquium, Bergische Universität Wuppertal, April 7.

60. O. Klein, *Numerical simulation of the use of traveling magnetic fields to stabilize crystal growth from the melt*, Warsaw Seminar on Industrial Mathematics (WSIM'10), March 18–19, Warsaw University of Technology, Poland, March 18.

61. D. Knees, *On the vanishing viscosity method in fracture mechanics*, Seminar Technomathematik, Technische Universität Graz, Institut für Numerische Mathematik, Austria, February 25.

62. ———, *On the vanishing viscosity method in fracture mechanics*, Berlin-Leipzig Seminar on Analysis and Probability Theory, Technische Universität Berlin, Institut für Mathematik, July 9.

63. ———, *Numerical convergence analysis for a vanishing viscosity model in fracture mechanics*, Workshop "Rate-independent Systems: Modeling, Analysis, and Computations", August 30 – September 3, Banff International Research Station for Mathematical Innovation and Discovery (BIRS), Canada, September 2.

64. W. König, *The parabolic Anderson model*, XIV Escola Brasileira de Probabilidade, August 2–7, Instituto Nacional de Matemática Pura e Aplicada (IMPA), Rio de Janeiro, Brazil.

65. ———, *Ordered random walks*, Augsburger Mathematisches Kolloquium, Universität Augsburg, Institut für Mathematik, January 26.

66. ———, *Phase transitions for dilute particle systems with Lennard–Jones potential*, University of Bath, Department of Mathematical Sciences, UK, April 14.

67. ———, *Ordered random walks*, Mathematisches Kolloquium der Universität Trier, Fachbereich Mathematik, April 29.

68. ———, *Die Universalitätsklassen im parabolischen Anderson-Modell*, Mathematisches Kolloquium, Technische Universität Darmstadt, Fachbereich Mathematik, July 7.

69. ———, *On random matrix theory*, Introductory Course for the IRTG Summer School Pro*Doc/IRTG Berlin-Zürich "Stochastic Models of Complex Processes" (Disentis, Switzerland, July 26–30, 2010), July 21–22, Technische Universität Berlin, July 21.

70. ———, *Phase transitions for dilute particle systems with Lennard–Jones potential*, Università di Roma "Tor Vergata", Dipartimento di Matematica, Italy, November 17.

71. ———, *Upper tails of self-intersection local times of random walks: Survey of proof techniques*, Excess Self-Intersection Local Times and Related Topics, December 6–10, Université de Marseille, Centre International de Rencontres Mathématiques (CIRM), France, December 7.

72. M. Korzec, *Modeling, model reduction, analysis and simulation of the self-assembly of thin crystalline nanostructures*, Seminar Prof. P. Rybka, Warsaw University, Institute of Applied Mathematics and Mechanics, Poland, May 6.

73. N. Krämer, *Conjugate gradient regularization — A statistical framework for partial least squares regression*, 4th Workshop on Partial Least Squares and Related Methods for Cutting-edge Research in Experimental Sciences, May 10–11, École Supérieure d'Électricité, Department of Information Systems and Decision Sciences, Gif-sur-Yvette, France, May 11.

74. N. Krämer, *Modeling of high-dimensional data with partial least squares*, University of Leeds, Faculty of Medicine and Health, Leeds Institute of Genetics, Health and Therapeutics, UK, September 2.

75. ———, *Regularized estimation of large-scale gene associaton networks*, 55. GMDS-Jahrestagung: Effiziente und wirtschaftliche Gesundheitsversorgung von heute und morgen — nur mit Medizinischer Dokumentation, Medizinischer Informatik, Medizinischer Biometrie und Epidemiologie, September 6–7, Hochschule Mannheim, Institut für Medizinische Informatik, September 6.

76. V. Krätschmer, *Nichtparametrische Schätzung verteilungsinvarianter Risikomaße*, Heinrich Heine Universität Düsseldorf, Institut für Mathematik, April 23.

77. ———, *Nichtparametrische Schätzung verteilungsinvarianter Risikomaße*, Universität Mannheim, Institut für Mathematik und Informatik, May 4.

78. ———, *Nichtparametrische Schätzung verteilungsinvarianter Risikomaße*, Universität Bayreuth, Fachbereich Mathematik, July 27.

79. ———, *Nichtparametrische Schätzung von verteilungsinvarianten Risikomaßen*, Mathematisches Kolloquium, Universität Duisburg-Essen, Fakultät für Mathematik, October 19.

80. K. Krumbiegel, *Sufficient optimality conditions for the Moreau–Yosida type regularization concept applied to state constrained problems*, Gemeinsame Jahrestagung Deutsche Mathematiker-Vereinigung (DMV) und Gesellschaft für Didaktik der Mathematik (GDM), March 8–12, Ludwig-Maximilians-Universität München, March 10.

81. ———, *Numerical analysis for elliptic Neumann boundary control problems with pointwise state and control constraints*, Technische Universität Dresden, Institut für Numerische Mathematik, May 11.

82. ———, *On the convergence and second order sufficient optimality conditions of the virtual control concept for semilinear state constrained optimal control problems*, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, May 18.

83. M. Lichtner, *Stability of delay differential equations with large delay*, Dynamical System Seminar, Portsmouth University, Department of Mathematics, UK, March 17.

84. M. Liero, *Rate-independent Kurzweil processes*, Workshop "Rate-independent Systems: Modeling, Analysis, and Computations", August 30 – September 3, Banff International Research Station for Mathematical Innovation and Discovery (BIRS), Canada, September 3.

85. A. Linke, *The problem of weak mass conservation in the discretization of the incompressible Navier–Stokes equations*, Université Blaise Pascal, Clermont-Ferrand II, France, July 13.

86. ———, *Zum Problem der Massenerhaltung bei der Diskretisierung inkompressibler Strömungen*, Ruhr-Universität Bochum, Fakultät für Mathematik, December 8.

87. ———, *Zum Problem der Massenerhaltung bei der Diskretisierung inkompressibler Strömungen*, Brandenburgische Technische Universität Cottbus, Fakultät 1 für Mathematik, Naturwissenschaften und Informatik, December 10.

88. R.L. Loeffen, *Absolute ruin in the insurance risk model of Ornstein–Uhlenbeck type*, 24th European Conference on Operational Research (EURO XXIV LISBON), July 11–14, Universidade de Lisboa, Faculdade de Ciéncias, Portugal, July 14.

89. ———, *The Ornstein–Uhlenbeck type risk model: Absolute ruin and spectral representation*, Talks in Actuarial Sciences, Université Libre de Bruxelles, Département de Mathématiques, Belgium, November 18.

90. P. Mathé, *Warum und wie rechnen wir mit allgemeinen Quelldarstellungen?*, Seminar Inverse Probleme (Fr. C. Böckmann), Universität Potsdam, Institut für Mathematik, January 12.

91. ———, *The Lepskii balancing principle for conjugate gradient regularization*, Workshop on Inverse Problems: Developments in Theory and Applications (IP-TA 2010), February 8–12, Stefan Banach International Mathematical Center, Warsaw, Poland, February 9.

92. ———, *Analysis of inverse problems under general smoothness assumptions*, 5th International Conference on Inverse Problems: Modeling and Simulation, May 24–29, Izmir University, Department of Mathematics and Computer Sciences, Antalya, Turkey, May 25.

93. B. Metzger, *The parabolic Anderson model: The asymptotics of the statistical moments and Lifshitz tails revisited*, EURANDOM, Eindhoven, The Netherlands, December 1.

94. A. Mielke, *Geometrische Nichtlinearitäten und Lie-Gruppen in der Elastoplastizität*, Mathematisches Kolloquium, Technische Universität Darmstadt, Fachbereich Mathematik, January 27.

95. ———, *Rate-independent plasticity as Gamma limit of a slow viscous gradient flow for wiggly energies*, Partial Differential Equations Seminar, University of Oxford & Queen's College, Centre for Nonlinear PDE, UK, February 22.

96. ———, *Gradient structures for reaction-diffusion systems and semiconductor equations*, 81th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2010), Session on Applied Analysis, March 22–26, Universität Karlsruhe, March 24.

97. ———, *Approaches to finite-strain elastoplasticity*, SIAM Conference on Mathematical Aspects of Materials Science (MS10), May 23–26, Philadelphia, USA, May 23.

98. ———, *A mathematical model for the evolution of microstructures in elastoplasticity*, Fifth International Conference on Multiscale Materials Modeling, Symposium on Mathematical Methods, October 4–8, Fraunhofer Institut für Werkstoffmechanik (IWM), Freiburg, October 4.

99. ———, *Gradient structures for reaction-diffusion systems and semiconductor models with interface dynamics*, International Conference on Evolution Equations, October 11–14, Technische Universität Darmstadt, Fachbereich Mathematik, Schmitten, October 12.

100. ———, *Rate-independent plasticity as Gamma limit of a slow viscous gradient flow for wiggly energies*, Nečas Seminar on Continuum Mechanics, Jindrich Nečas Center for Mathematical Modeling, Prague, Czech Republic, November 8.

101. ———, *Rate-independent plasticity as Gamma limit of a slow viscous gradient flow for wiggly discrete energy*, Zwei-Städte-Kolloquium zur Analysis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Fachbereich Mathematik, November 26.

102. H.-J. Mucha, *Automatische Klassifikation (Clusteranalyse)*, IBM SPSS Kundentag 2010, June 8, SPSS GmbH Software, München, June 8.

103. ———, *Pairwise data clustering accompanied by validation and visualisation*, 3rd German-Japanese Workshop "Advances in Data Analysis and Related New Techniques and Applications", July 20–21, Karlsruhe Institute of Technology (KIT), July 20.

104. ———, *An accelerated K-means algorithm based on adaptive distances*, 34th Annual Conference of the German Classification Society (GfKl) and International Symposium on the Data Analysis Interface, July 21–23, Karlsruhe Institute of Technology (KIT), July 22.

105. ———, *Visualisation of cluster analysis results*, Joint Meeting GfKl (German Classification Society) — CLADAG 2010, September 6–10, University of Florence, Department of Statistics, Italy, September 9.

106. H. Neidhardt, *Scattering for self-adjoint extensions*, Analysis Seminar, Aalborg University, Department of Mathematical Sciences, Denmark, April 22.

107. ———, *On the unitary equivalence of absolutely continuous parts of self-adjoint extensions*, 21th International Workshop on Operator Theory and Applications (IWOTA 2010), Session "Extension Theory and Applications", July 12–16, Technische Universität Berlin, Institut für Mathematik, July 15.

108. ———, *On perturbation determinants for non-selfadjoint operators*, ESF Exploratory Workshop on Mathematical Aspects of the Physics with Non-Self-Adjoint Operators, August 30 – September 3, Czech Academy of Sciences, Nuclear Physics Institute, Prague, September 1.

109. ———, *Scattering matrices and Weyl function*, Research seminar of the Graduate School of Natural Science and Technology, Okayama University, Department of Mathematics, Japan, September 14.

110. ———, *The contribution of Takashi to Trotter–Kato product formulas for imaginary times*, Symposium dedicated to Takashi Ichinose's 70th birthday, Kanazawa University, Faculty of Science, Department of Mathematics, Japan, September 17.

111. ———, *Extensions, perturbation determinants and trace formulas*, Workshop on Systems & Operators in Honor of Henk de Snoo, December 14–17, University of Groningen, Faculty of Mathematics and Natural Sciences, The Netherlands, December 16.

112. O.E. Omel'chenko, *On the dynamical nature of chimera states*, The 8th AIMS International Conference on Dynamical Systems, Differential Equations and Applications, May 25–28, Technische Universität Dresden, May 25.

113. ———, *Moving chimera states*, International Workshop "Nonlinear Dynamics on Networks", July 5–9, National Academy of Sciences of Ukraine, Kiev, July 6.

114. ———, *Dynamical properties of chimera states*, Dynamics Days Europe, September 6–10, University of Bristol, Department of Engineering Mathematics, UK, September 6.

115. A. Petrov, *On a 3D model for shape-memory alloys*, Workshop "Rate-independent Systems: Modeling, Analysis, and Computations", August 30 – September 3, Banff International Research Station for Mathematical Innovation and Discovery (BIRS), Canada, September 2.

116. J. Polzehl, *Medical image analysis for structural and functional MRI*, The R User Conference 2010, July 20–23, National Institute of Standards and Technology (NIST), Gaithersburg, USA, July 20.

117. ———, *Structural adaptive smoothing in neuroscience applications*, Statistische Woche Nürnberg 2010, September 14–17, Friedrich-Alexander-Universität Erlangen-Nürnberg, Naturwissenschaftliche Fakultät, September 16.

118. P.N. Racec, *Scattering in cylindrical nanowire heterostructures: R-matrix formalism and finite element method*, University of Iceland, Science Institute, Icelandic Center of Computational Science, Reykjavik, August 18.

119. M. Radziunas, *Modeling, simulation and analysis of nonlinear dynamics in multisection semiconductor lasers*, 15th International Conference "Mathematical Modelling and Analysis" (MMA2010), May 26–29, Druskininkai, Lithuania, May 29.

120. A. Rathsfeld, *Numerical reconstruction of elastic obstacles from the far-field data of scattered acoustic waves*, Workshop on Inverse Problems for Waves: Methods and Applications, March 29–30, Ecole Polytechnique, Palaiseau, France, March 29.

121. J. Rehberg, *L^∞ -estimates for fractional resolvent powers*, 21th International Workshop on Operator Theory and Applications (IWOTA 2010), Session "Spectral Theory and Evolution Equations", July 12–16, Technische Universität Berlin, Institut für Mathematik, July 13.

122. ———, *On parabolic equations with non-homogeneous Neumann boundary conditions*, International Conference on Evolution Equations, October 11–14, Technische Universität Darmstadt, Fachbereich Mathematik, Schmitten, October 11.

123. O. Rott, *An iterative method for the multipliers of periodic delay-differential equations and the analysis of a PDE milling model*, 9th IFAC Workshop on Time Delay Systems, June 7–9, Czech Technical University, Prague, Czech Republic, June 8.

124. ———, *Analysis of uncertainties in the stability prediction for milling processes*, 2nd International Conference "Process Machine Interactions", June 10–11, The University of British Columbia, Vancouver, Canada, June 11.

125. G. Schmidt, *Integral methods for conical diffraction by multi-profile gratings*, Annual International Conference "Days on Diffraction 2010", June 8–11, St. Petersburg, Russia, June 9.

126. ———, *Fast computation of high-dimensional volume potentials*, Trilateral Workshop on Separation of Variables and Applications (SVA), September 8–10, La Colle-sur-Loup, France, September 10.

127. ———, *On the computation of volume potentials over high-dimensional rectangular domains*, The First Workshop on Approximate Approximations and Their Applications, December 14–15, University of Liverpool, UK, December 15.

128. J.G.M. Schoenmakers, *Advanced Libor modeling*, Postbank Bonn, February 25.

129. ———, *Holomorphic transforms with application to affine processes*, 5th General Conference in Advanced Mathematical Methods in Finance, May 4–8, University of Ljubljana, Faculty of Mathematics and Physics, Slovenia, May 6.

130. ———, *On three innovations in financial modeling*, Colloquium, University of Twente, Faculty of Electrical Engineering, Mathematics and Computer Science, The Netherlands, August 24.

131. H. Si, *TetGen, a Delaunay tetrahedral mesh generator*, Massachusetts Institute of Technology, Department of Aeronautics & Astronautics, Cambridge, USA, October 1.

132. ———, *3D boundary conforming Delaunay mesh generation*, Carnegie Mellon University, Pittsburgh, USA, October 7.

133. V. Spokoiny, *Local parametric estimation*, 4 talks, October 18–22, École Nationale de la Statistique et de l'Analyse de l'Information (ENSAI), Rennes, France.

134. ———, *Sparse non-Gaussian component analysis*, University of Cambridge, Faculty of Mathematics, Statistical Laboratory, UK, May 7.

135. ———, *Semidefinite non-Gaussian component analysis*, Bivariate Penalty Choice in Model Selection, Deutsches Diabetes Zentrum Düsseldorf, June 17.

136. ———, *Sparse non-Gaussian component analysis*, Journées STAR 2010, October 21–22, Université Rennes II, France, October 22.

137. ———, *Semidefinite optimization in instrumental variable estimation with shape constraints*, Conference on "Shape Restrictions in Non- and Semiparametric Estimation of Econometric Models", November 1–7, Northwestern University, Department of Statisics, Chicago, USA, November 6.

138. ———, *Sparse non-Gaussian component analysis*, School of Mathematics Colloquium, November 19, University of Edinburgh, School of Mathematics, UK, November 19.

139. ———, *Statistical estimation: Modern view*, Rencontres de Statistiques Mathématiques 10, December 13–17, Centre International de Rencontres Mathématiques (CIRM), Luminy, France, December 15.

140. ———, *Statistical estimation: Modern view*, Rencontres de Statistiques Mathématiques 10, December 13–17, Centre International de Rencontres Mathématiques (CIRM), Luminy, France, December 16.

141. J. Sprekels, *Introduction to Optimal Control Problems for PDEs (mini-course)*, 4 talks, Summer School "Optimal Control of Partial Differential Equations", July 12–17, Cortona, Italy.

142. ———, *Praktische und mathematische Probleme bei der Züchtung von Halbleiter-Einkristallen*, Technische Universität Chemnitz, Forschungsseminar Numerik, January 5.

143. ———, *Technical and mathematical problems in the Czochralski growth of single crystals*, Workshop "New Directions in Simulation, Control and Analysis for Interfaces and Free Boundaries", January 31 – February 6, Mathematisches Forschungsinstitut Oberwolfach, February 1.

144. H. Stephan, *Asymptotisches Verhalten positiver Halbgruppen*, Oberseminar Analysis, Technische Universität Dresden, Institut für Analysis, January 14.

145. ———, *Evolution equations conserving positivity*, Colloquium of Centre for Analysis, Scientific Computing and Applications (CASA), Technische Universiteit Einhoven, The Netherlands, April 21.

146. K. Tabelow, *Structural adaptive smoothing fMRI and DTI data*, Workshop on Novel Reconstruction Strategies in NMR and MRI 2010, September 9–11, Georg-August-Universität Göttingen, Fakultät für Mathematik und Informatik, September 11.

147. M. Thomas, *From damage to delamination in nonlinearly elastic materials at small strains*, Workshop "Microstructures in Solids: From Quantum Models to Continua", March 14–20, Mathematisches Forschungsinstitut Oberwolfach, March 18.

148. M. Thomas, *Rate-independent damage and delamination processes*, Workshop "Rate-independent Systems: Modeling, Analysis, and Computations", August 30 – September 3, Banff International Research Station for Mathematical Innovation and Discovery (BIRS), Canada, August 31.

149. V.Z. Tronciu, *Semiconductor laser a key element for new generation optoelectronic systems*, The 3rd International Conference on Telecommunications, Electronics and Informatics (ICTEI 2010), May 20–23, Technical University of Moldova, Chisinau, Moldova, May 21.

150. ———, *Chaos based communication using multi-section semiconductor laser*, École Polytechnique Fédérale de Lausanne (EPFL-SB), Laboratory of Physics of Nanostructures, Switzerland, September 9.

151. ———, *Nonlinear dynamics in semiconductor lasers — Theory and experiments*, Vrije Universiteit Brussel, Department of Applied Physics and Photonics, Belgium, September 16.

152. V.Z. Tronciu, C. Fiebig, M. Lichtner, H. Wenzel, *Numerical and experimental investigations of DBR tapered lasers*, The 3rd International Conference on Telecommunications, Electronics and Informatics (ICTEI 2010), May 20–23, Technical University of Moldova, Chisinau, Moldova, May 20.

153. A.G. Vladimirov, *Nonlinear dynamics in lasers*, Technische Universität Berlin, Institut für Festkörperphysik, March 24.

154. ———, *Interaction of dissipative solitons and pulses in laser systems*, Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Belgium, April 21.

155. ———, *Localized structures of light and their interaction*, Imperial College London, Department of Applied Mathematics, UK, April 27.

156. ———, *Introduction to mode-locking in lasers*, Graduate College of the Collaborative Research Center SFB 787 "Semiconductor Nanophotonics: Materials, Models, Devices", May 9–11, Technische Universität Berlin, Institut für Festkörperphysik, Graal-Müritz, May 10.

157. B. Wagner, *Spincoating of evaporating polymer solutions*, Workshop on Mathematical Models in Photovoltaic Devices, University of Southampton, UK, September 23.

158. B. Wagner, R. Seemann, *Mathematical modeling, analysis, numerical simulation of thin liquid bilayers and validation experiments*, Kick-off Meeting of DFG Priority Program 1506 "Transport Processes at Fluidic Interfaces", Technische Universität Darmstadt, Center of Smart Interfaces, July 7.

159. W. Wagner, *Kinetic equations and Markov jump processes*, Isaac Newton Institute for Mathematical Sciences, Programme: Partial Differential Equations in Kinetic Theories, Cambridge, UK, November 29.

160. M. Wolfrum, *Scaling properties of the spectrum for ODEs with large delay*, 8th AIMS International Conference on Dynamical Systems, Differential Equations and Applications, May 25–28, Technische Universität Dresden, May 25.

161. ———, *Chimera states are chaotic transients*, International Workshop "Nonlinear Dynamics on Networks", July 5–9, National Academy of Sciences of Ukraine, Kiev, July 6.

162. ———, *Scaling properties of the spectrum for DDEs with large delay*, Applied Maths Seminar, University of Exeter, Institute of Applied Mathematics, UK, November 22.

A.8.3 Talks for a More General Public

1. C. Guhlke, *Luftballons, Lithium-Ionen-Batterien und Wasserstoffautos — Ein Fall für die Mathematik!*, MathInside — Mathematik ist überall, Urania, Berlin, November 2.

2. ———, *Ein Fall für die Mathematik!*, 67. Konferenz der deutschsprachigen Mathematikfachschaften (KoMa 2010), Universität Magdeburg, November 26.

3. ———, *Luftballons, Lithium-Ionen-Batterien und Wasserstoffautos — Ein Fall für die Mathematik!*, DFG Research Center Matheon: Rent The Center, Heinrich-Schliemann-Gymnasium, Berlin, December 1.

4. R. Huth, *Keine Schlüsseltechnologien ohne Mathematik*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2010, WIAS, June 5.

5. W. König, *Erfolgsgeschichte eines stochastischen Prozesses: Die Brown'sche Bewegung*, 15. Berliner Tag der Mathematik (15th Berlin Day of Mathematics), Technische Universität Berlin, May 8.

6. ———, *Die Anfänge der Wahrscheinlichkeitsrechnung als Wissenschaft*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2010, WIAS, June 5.

7. ———, *Streifzüge durch die Entwicklung der Wahrscheinlichkeitstheorie*, MathInside — Mathematik ist überall, Urania, Berlin, November 9.

8. N. Krämer, *How to write a good paper*, Technische Universität Berlin, Institute for Software Engineering and Theoretical Computer Science, April 14.

9. G. Reinhardt, *Abbildungen von 3D-Objekten auf 2D-Flächen — Computerspiele gehen nicht ohne diese*, 15. Berliner Tag der Mathematik (15th Berlin Day of Mathematics), Technische Universität Berlin, May 8.

10. M. Thomas, *Vom Hooke'schen Gesetz zu schlauen Materialien*, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2010, WIAS, June 5.

Long Night of the Sciences at WIAS on June 5, 2010

A.8.4 Posters

1. P. Friz, *A (rough) pathwise approach to a class of non-linear stochastic partial diffenrential equations*, Workshop "Stochastic Partial Differential Equations (SPDEs)", Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, January 4–6.
2. A. Beinrucker, *MASH — Massive sets of heuristics*, Machine Learning Summer School, Canberra, Australia, September 27 – October 6.
3. G. Blanchard, N. Krämer, *Kernel partial least squares is universally consistent*, AI & Statistics 2010, Sardinia, Italy, May 13–15.
4. ———, *Optimal rates for conjugate gradient regularization*, AI & Statistics 2010, Sardinia, Italy, May 13–15.
5. W. Dreyer, P.-É. Druet, F. Duderstadt, Ch. Grützmacher, O. Klein, D. Reinhardt, J. Sprekels, Ch. Frank-Rotsch, F.-M. Kiessling, W. Miller, U. Rehse, P. Rudolph, Ch. Lechner, *Crystal growth under the influence of traveling magnetic fields*, Status Seminar AVANT*SOLAR*, Griebnitzsee, September 9–10.
6. K. Afanasiev, F. Duderstadt, W. Dreyer, St. Eichler, O. Klein, J. Sprekels, *On effects in the vicinity of the solid melt interface during GaAs crystal growth from the melt*, Status Seminar AVANT*SOLAR*, Griebnitzsee, September 9–10.

7. J. Fuhrmann, A. Fiebach, G.P. Patsis, *Macroscopic and stochastic modeling approaches to pattern doubling by acid catalyzed cross-linking*, Workshop "SPIE Advanced Lithography", San Jose, California, USA, February 21–25.

8. K. Gärtner, H. Si, *We like Delaunay grids — Why?*, The Third International Workshop on Grid Generation for Numerical Computations (Tetrahedron Workshop III), Swansea University, UK, September 14–15.

9. D. Hömberg, F. Hoffmann, R.H. Hoppe, A. Schmidt, *Modellierung, Simulation und Optimierung des Mehrfrequenzverfahrens für die induktive Wärmebehandlung als Bestandteil der modernen Fertigung*, BMBF Status Seminar "Mathematik für Innovationen in Industrie und Dienstleistung", Kaiserslautern, June 9–10.

10. S. Jansen, M. Aizenman, P. Jung, *Symmetry breaking in quasi 1D Coulomb systems*, Combinatorics and Analysis in Spatial Probability — ESF Mathematics Conference in Partnership with EMS and ERCOM, Eindhoven, The Netherlands, December 12–18.

11. V. John, O.C. Suciu, *SimParTurS: Gekoppelte Simulationen von Partikelpopulationen*, BMBF Status Seminar "Mathematik für Innovationen in Industrie und Dienstleistungen", Kaiserslautern, June 9.

12. O. Klein, K. Afanasiev, F. Duderstadt, W. Dreyer, St. Eichler, J. Sprekels, *On effects in the vicinity of the solid melt interface during crystal growth from the melt*, The 16th International Conference on Crystal Growth (ICCG-16) in conjunction with The 14th International Conference on Vapor Growth and Epitaxy (ICVGE-14), Beijing, China, August 8–13.

13. M. Sander, R.I.A. Patterson, A. Braumann, A. Rai, M. Kraft, *Boundary value stochastic particle methods for population balance problems*, 4th International Conference on Population Balance Modelling (PBM 2010), Berlin, September 15–17.

14. J. Polzehl, K. Tabelow, *Image and signal processing in the biomedical sciences: Diffusion-weighted imaging modeling and beyond*, 1st Annual Scientific Symposium "Ultrahigh Field Magnetic Resonance", Max Delbrück Center, Berlin, April 16.

15. E. Schmeyer, V. John, R. Bordás, D. Thévenin, *Referenzexperimente im Windkanal, numerische Simulation und Validierung*, Annual Meeting 2010 of DFG Priority Program 1276 MetStröm, Zuse Institute Berlin, October 28–29.

16. K. Tabelow, J.D. Clayden, P. Lafayede Micheaux, J. Polzehl, V.J. Schmid, B. Whitcher, *Image analysis and statistical inference in NeuroImaging with R.*, Human Brain Mapping 2010, Barcelona, Spain, June 6–10.

17. K. Tabelow, J. Polzehl, S. Mohammadi, M. Deppe, *Impact of smoothing on the interpretation of FA maps*, Human Brain Mapping 2010, Barcelona, Spain, June 6–10.

18. V.Z. Tronciu, S.S. Rusu, C. Pîrtac, *Dynamics of coupled semiconductor lasers. On/off phase shift keying encription method*, The 3rd International Conference on Telecommunications, Electronics and Informatics (ICTEI 2010), Chisinau, Moldova, May 20–23.

19. B. Wagner, A. Münch, K. Afanasiev, D. Peschka, *The role of slippage in thin liquid films and droplets on rigid and viscoelastic substrates*, Workshop of the DFG Priority Program 1164 "Nano- & Microfluidics", Norderney, February 22–26.

The Berlin Senator for Economics, Technology and Women's Issues, Harald Wolf, visits the WIAS presentation at the Leibniz Association's booth at the *Hannover Industriemesse 2010* (Hannover Industrial Fair 2010)

A.8.5 Contributions to Exhibitions

1. F. Anker, *Ein Überblick über WIAS-Entwicklungen auf dem Gebiet der Software*, Hannover Industriemesse 2010, April 19–21.
2. R. Nürnberg, *WIAS-TeSCA*, Hannover Industriemesse 2010, April 22.
3. M. Radziunas, *LDSL-tool*, Hannover Industriemesse 2010, April 23.
4. T. Streckenbach, *Presentation of TetGen and WIAS-SHarP*, Hannover Industriemesse 2010, April 22–23.

A.9 Visits to other Institutions[7]

1. M. Becker, Universität Leipzig, Mathematisches Institut, March 24–29.
2. A. Beinrucker, Australian National University, School of Computer Science, Canberra, September 27 – October 6.
3. A. Caiazzo, Institut National de Recherche en Informatique et Automatique (INRIA), REO, Paris, France, July 12–23.
4. ———, Institut National de Recherche en Informatique et Automatique (INRIA), REO, Paris, France, December 9–13.
5. W. Dreyer, Technische Universität Darmstadt, Center of Smart Interfaces, April 26–29.
6. F. Duderstadt, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, February 1–5.
7. J. Elschner, University of Tokyo, Department of Mathematical Sciences, Japan, March 8–26.
8. J. Fuhrmann, Université Blaise Pascal, Clermont-Ferrand II, France, June 7–11.
9. T. Girnyk, École Polytechnique Fédérale de Lausanne, Laboratory of Nonlinear Systems (EPFL-LANOS), Switzerland, November 13–21.
10. K. Hoke, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, April 25 – May 2.
11. D. Hömberg, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, March 15–26.
12. ———, Nippon Steel Corporation, Chiba, Japan, September 4–10.
13. ———, University of Tokyo, Graduate School of Mathematical Sciences, Japan, October 25–29.
14. S. Jansen, Università di Roma "Tor Vergata", Dipartimento di Matematica, Italy, November 13, 2010 – January 21, 2011.
15. V. John, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain, February 22–26.
16. D. Knees, Università degli Studi di Udine, Dipartimento di Matematica e Informatica, Italy, January 31 – February 6.
17. ———, Technische Universität Graz, Institut für Numerische Mathematik, Austria, February 21–26.
18. ———, Universität Erlangen, Lehrstuhl für Angewandte Mathematik, July 19–22.
19. ———, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche (IMATI-CNR), Pavia, Italy, November 22–26.
20. W. König, University of Bath, Department of Mathematical Sciences, UK, April 12–17.
21. ———, Università di Roma "Tor Vergata" Dipartimento di Matematica, Italy, November 15–22.
22. K. Krumbiegel, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, May 17–21.
23. M. Lichtner, Portsmouth University, Department of Mathematics, UK, March 16–19.
24. M. Liero, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche (IMATI-CNR), Pavia, Italy, November 28 – December 1.
25. A. Linke, Université Blaise Pascal, Clermont-Ferrand II, France, July 12–16.

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

26. R.L. Loeffen, Université Libre de Bruxelles, Département de Mathématique, Service Sciences Actuarielles, ECARES, Belgium, February 1 – March 4.
27. ———, Université Libre de Bruxelles, Département de Mathématique and ECARES, Belgium, March 22 – April 16.
28. ———, University of Wroclaw, Mathematical Institute, Poland, September 11–18.
29. ———, Université Libre de Bruxelles, Département de Mathématique, Belgium, November 8 – December 4.
30. ———, University of Oxford, Department of Statistics, UK, December 7–10.
31. B. Metzger, EURANDOM, Eindhoven, The Netherlands, November 29 – December 3.
32. A. Mielke, University of Oxford & Queen's College, Centre for Nonlinear PDE, UK, February 21–26.
33. ———, Charles University/Jindrich Nečas Center for Mathematical Modeling, Prague, Czech Republic, November 3–25.
34. H. Neidhardt, Aalborg University, Department of Mathematical Sciences, Denmark, April 19–23.
35. D. Peschka, University of California, Department of Mathematics, Los Angeles, USA, July 12 – October 16.
36. Th. Petzold, Nippon Steel Corporation, Tokyo, Japan, September 4–10.
37. J. Polzehl, University of Minnesota, School of Statistics, Minneapolis, USA, July 9–16.
38. P.N. Racec, University of Iceland, Science Institute, Center of Computational Science, Reykjavik, Iceland, July 26–30.
39. S. Reichelt, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche (IMATI-CNR), Pavia, Italy, November 22–26.
40. V. Spokoiny, National University of Singapore, Department of Statistics and Applied Probability, Singapore, March 1–10.
41. ———, École Nationale de la Statistique et de l'Analyse de l'Information (ENSAI), Rennes, France, October 18–22.
42. J. Sprekels, Università di Pavia, Dipartimento di Matematica "F. Casorati"/Istituto di Matematica Applicata e Tecnologie Informatiche, Italy, September 13–24.
43. H. Stephan, Eindhoven University of Technology, Department of Mathematics and Computer Science, The Netherlands, April 19–23.
44. A.G. Vladimirov, Université Libre de Bruxelles, Faculté de Science, Optique Nonlinéaire Théorique (ONT), Belgium, April 16–24.
45. ———, Imperial College London, Department of Applied Mathematics, UK, April 24–29.
46. ———, University College Cork, Tyndall National Institute, Ireland, December 2–13.
47. B. Wagner, University of Oxford, Oxford Centre for Collaborative Applied Mathematics, UK, February 8–12.
48. ———, University of Oxford, Oxford Centre for Collaborative Applied Mathematics, UK, March 15–29.
49. ———, University of Oxford, Oxford Centre for Collaborative Applied Mathematics, UK, April 7–23.
50. ———, University of Oxford, Oxford Centre for Collaborative Applied Mathematics, UK, August 21 – October 1.
51. ———, University of Oxford, Oxford Centre for Collaborative Applied Mathematics, UK, November 15–19.
52. W. Wagner, Isaac Newton Institute for Mathematical Sciences, Programme: Partial Differential Equations in Kinetic Theories, Cambridge, UK, September 27 – December 17.
53. M. Wolfrum, University of Exeter, Institute of Applied Mathematics, UK, November 21–24.

A.10 Academic Teaching[8]

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), Technische Universität 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. W. König, *Stochastische Modelle* (lecture), Technische Universität Berlin, 4 SWS.
13. J. Blath, J. Gärtner, W. König, N. Kurt, *Stochastic Models in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
14. J.-D. Deuschel, P. Friz, J. Gärtner, P. Imkeller, W. König, U. Küchler, H. Föllmer, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS Berlin, 2 SWS.
15. V. Krätschmer, *Selected Topics in Banking and Insurance* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
16. M. Lichtner, *Fourieranalysis* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
17. P. Mathé, *Statistische Datenanalyse mit R* (seminar), Freie Universität Berlin, 2 SWS.
18. A. Mielke, *Variationsrechnung* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
19. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin, 2 SWS.
20. V. Spokoiny, *Nichtparametrische Verfahren* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
21. V. Spokoiny, W. Härdle, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
22. J. Sprekels, *Höhere Analysis I (Funktionalanalysis)/BMS Basic Course "Functional Analysis"* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
23. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
24. M. Wolfrum, B. Fiedler, St. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS/Freie Universität Berlin, 2 SWS.

[8] SWS = semester periods per week

Summer Semester 2010

1. P. Friz, *Finanzmathematik II* (lecture), Technische Universität Berlin, 4 SWS.
2. ———, *Finanzmathematik II* (practice), Technische Universität Berlin, 2 SWS.
3. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS, 2 SWS.
4. M. Becker, *Wahrscheinlichkeitstheorie für Lehramt* (seminar), Universität Leipzig, 2 SWS.
5. R. Henrion, W. Römisch, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
6. D. Hömberg, *Optimalsteuerung bei partiellen Differentialgleichungen* (lecture), Technische Universität Berlin, 4 SWS.
7. ———, *Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
8. V. John, *Numerische Simulation konvektions-dominanter Probleme* (lecture), Technische Universität Berlin, 2 SWS.
9. ———, *Numerische Simulation konvektions-dominanter Probleme* (seminar), Technische Universität Berlin, 2 SWS.
10. ———, *Numerische Simulation konvektions-dominanter Probleme* (practice), Technische Universität Berlin, 2 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. J.-D. Deuschel, P. Friz, J. Gärtner, P. Imkeller, W. König, U. Küchler, H. Föllmer, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
13. V. Krätschmer, *Advanced Methods in Quantitative Finance* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
14. M. Lichtner, *Einführung in Evolutionsgleichungen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
15. A. Mielke, *Ausgewählte Themen der Variationsrechnung* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
16. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin, 2 SWS.
17. V. Spokoiny, *Nichtparametrische Verfahren* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
18. V. Spokoiny, W. Härdle, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
19. J. Sprekels, *Höhere Analysis II (Partielle Differentialgleichungen)/BMS Basic Course "Partial Differential Equations"* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
20. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
21. M. Wolfrum, B. Fiedler, St. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS/Freie Universität Berlin, 2 SWS.

Winter Semester 2010/2011

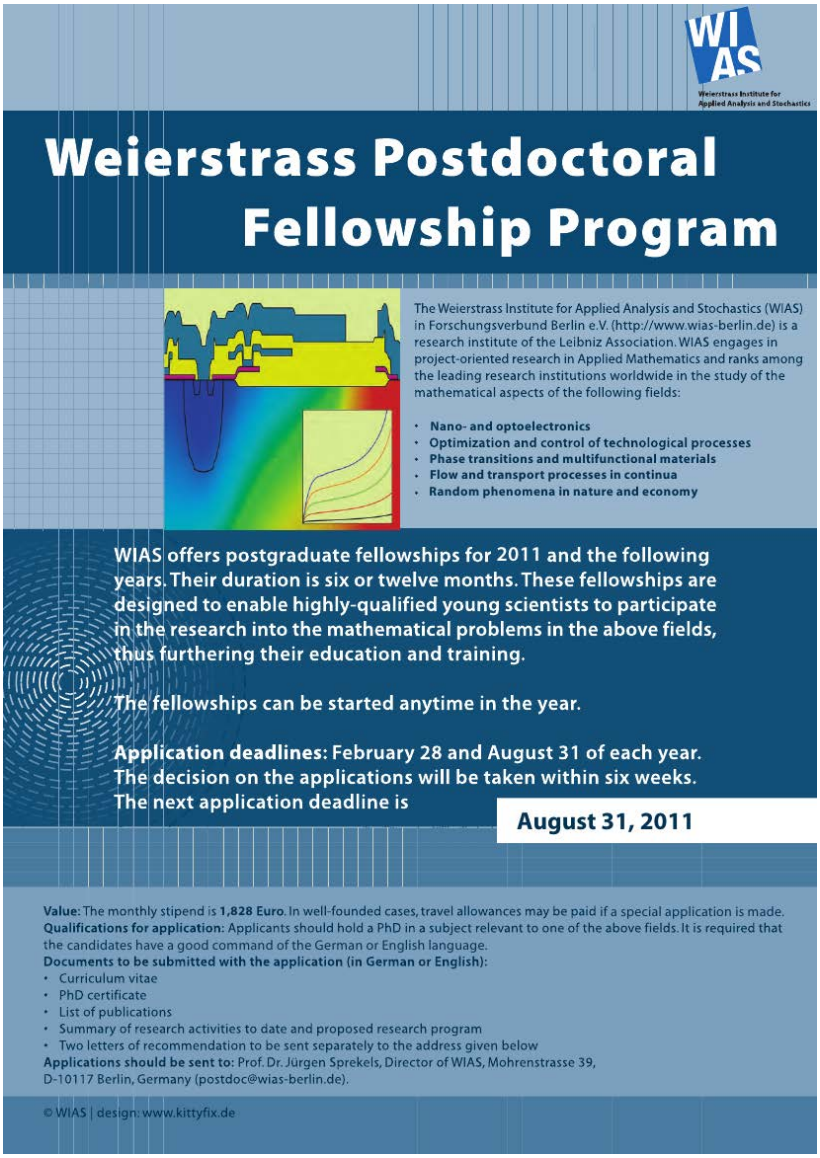
1. P. Friz, *Finanzmathematik I* (lecture), Technische Universität Berlin, 4 SWS.
2. ———, *Topics in Stochastic Analysis* (seminar), Technische Universität Berlin, 2 SWS.

3. ———, *Finanzmathematik I* (practice), Technische Universität Berlin, 2 SWS.
4. U. Bandelow, *Theorie photonischer Komponenten* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
5. ———, *Theorie photonischer Komponenten* (practice), Humboldt-Universität zu Berlin, 1 SWS.
6. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), Humboldt-Universität zu Berlin/WIAS Berlin, 2 SWS.
7. M. Becker, *Grundwissen Schulmathematik* (seminar), Universität Leipzig, 2 SWS.
8. D. Belomestny, *Simulationsbasierte Algorithmen für optimale Stopp- und Steuerungsprobleme* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
9. W. Dreyer, *Grundlagen der Kontinuumstheorie I/Tensoranalysis* (lecture), Technische Universität Berlin, 4 SWS.
10. P.-É. Druet, *Partielle Differentialgleichungen der Physik* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
11. A. Glitzky, *Einführung in die Kontrolltheorie und optimale Steuerung* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
12. R. Henrion, W. Römisch, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
13. D. Hömberg, *Nichtlineare Optimierung* (seminar), Technische Universität Berlin, 2 SWS.
14. V. John, A. Linke, *Numerik IVb: Simulation inkompressibler Strömungen* (lecture), Freie Universität Berlin, 2 SWS.
15. ———, *Numerik IVb: Simulation inkompressibler Strömungen* (seminar), Freie Universität Berlin, 2 SWS.
16. ———, *Numerik IVb: Simulation inkompressibler Strömungen* (practice), Freie Universität Berlin, 2 SWS.
17. 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.
18. O. Klein, *Mathematische Modellierung von Hysterese-Effekten* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
19. W. König, *Große Abweichungen* (lecture), Technische Universität Berlin, 4 SWS.
20. J.-D. Deuschel, P. Friz, J. Gärtner, P. Imkeller, W. König, U. Küchler, H. Föllmer, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), Technische Universität Berlin, 2 SWS.
21. V. Krätschmer, *Selected Topics in Banking and Insurance* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
22. Ch. Kraus, *Allgemeine Variationsmethoden I* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
23. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin, 2 SWS.
24. R. Müller, *Numerical Methods in Science and Technology* (lecture), Universität Bonn, 4 SWS.
25. J. Polzehl, K. Tabelow, *Anwendungen der Statistik* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
26. V. Spokoiny, *Nichtparametrische Verfahren* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
27. V. Spokoiny, M. Reiss, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
28. H. Stephan, *Anfänge der Analysis und euklidische Geometrie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
29. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
30. M. Wolfrum, B. Fiedler, St. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS Berlin/Freie Universität Berlin, 2 SWS.

A.11 Weierstrass Postdoctoral Fellowship Program

In 2005, the Weierstrass Institute 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.



A.12 Visiting Scientists[9]

A.12.1 Guests

1. St. Adams, University of Warwick, Mathematics Institute, Coventry, UK, May 10–18.
2. ———, September 1–21.
3. P. Alquier, Université Paris 7, Laboratoire de Probabilités et Modèles Aléatoires, France, November 30 – December 2.
4. U. Assmann, Universität Duisburg-Essen, Fachbereich Mathematik, September 27 – October 1.
5. G.R. Barrenechea, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, August 21 – September 3.
6. M. Biskup, University of California, Los Angeles, Department of Mathematics, USA, August 23 – September 3.
7. N. Bochkina, University of Edinburgh, The School of Mathematics, UK, June 20–28.
8. D. Bothe, Technische Universität Darmstadt, Center of Smart Interfaces, August 24–27.
9. O. Boyarkin, Universität Augsburg, Institut für Mathematik, November 1–26.
10. E. Burman, University of Sussex, Department of Mathematics, Brighton, UK, October 10–23.
11. C. Butucea, Université des Sciences et Technologies de Lille 1, Laboratoire Paul Painlevé, France, November 23–27.
12. Y. Chen, National University of Singapore, Department of Statistics and Applied Probability, July 19–23.
13. R. Čiegis, Vilnius Gediminas Technical University, Department of Mathematical Modeling, Lithuania, November 1–18.
14. S. Delattre, Université Paris 6, Laboratoire de Probabilités et Modèles Aléatoires, France, June 7–11.
15. A. Ern, Université Paris-Est, Centre d'Enseignement et de Recherche en Mathématiques et Calcul Scientifique (CERMICS), Marne la Vallée, France, October 10–21.
16. A. Faraj, Technische Universität Braunschweig, Institut für Analysis und Algebra, November 9–12.
17. A. Fiaschi, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche, Pavia, Italy, May 17–21.
18. J. Flemming, Technische Universität Chemnitz, Fakultät für Mathematik, July 26–30.
19. M. Gerdts, Universität Würzburg, Institut für Mathematik, August 16 – September 12.
20. J. Giesselmann, Universität Stuttgart, Fachbereich Mathematik, August 16–20.
21. T. Girnyk, National Taras Shevchenko University, Mechanics and Mathematics Faculty, Kiev, Ukraine, March 21–28.
22. D. Glazkov, Yaroslavl Demidov State University, Department of Mathematics, Russia, September 26 – October 9.
23. St. Grönneberg, University of Oslo, Department of Mathematics, Norway, January 4 – February 3.
24. R. Haller-Dintelmann, Technische Universität Darmstadt, Fachbereich Mathematik, August 23 – September 10.

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

25. ———, September 27 – October 1.
26. K. Hanowski, Freie Universität Berlin, Fachbereich Mathematik, July 19 – October 15.
27. E. Hoarau, Agence Nationale pour la Gestion des Déchets Radioactifs, Direction Scientifique, Service Colis et Matériaux, Chatenay-Malabry, France, January 17 – April 16.
28. ———, November 1–12.
29. J. Horowitz, Northwestern University, Department of Economics, Evanston, Illinois, USA, January 28–31.
30. I. Kashchenko, Yaroslavl Demidov State University, Department of Mathematics, Russia, November 6–14.
31. G. Kerkyacharin, Université Paris 7, Laboratoire de Probabilités et Modèles Aléatoires, France, November 16–18.
32. A. Khludnev, Russian Academy of Sciences, Lavrentyev Institute of Hydrodynamics, Novosibirsk, January 27 – February 1.
33. W. Kirsch, Fernuniversität Hagen, Fakultät für Mathematik und Informatik, Fachrichtung Mathematik, June 13–19.
34. P. Knobloch, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, August 5–25.
35. H. Kovařík, Politecnico di Torino, Dipartimento di Matematica, Italy, April 25–28.
36. M. Kraft, University of Cambridge, Department of Chemical Engineering, UK, August 22 – September 25.
37. P. Krejčí, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, October 18–31.
38. ———, November 15–28.
39. R.J.A. Laeven, Tilburg University, Department of Econometrics and Operations Research, The Netherlands, September 20 – October 1.
40. Y. Latushkin, University of Missouri, Department of Mathematics, Columbia, USA, July 12–17.
41. R. Liptser, Tel Aviv University, Department of Electrical Engineering — Systems, June 1 – July 1.
42. J. Liu, Southeast University, Department of Mathematics, Nanjing, Republic of China, July 13 – August 8.
43. O. Lopez, Université Paris 6, Laboratoire de Statistique Théorique et Appliquée (LSTA), France, January 25 – February 6.
44. ———, September 13–22.
45. V. Maistrenko, National Academy of Sciences of Ukraine, National Center for Medical and Biotechnical Research, Kiev, October 24–30.
46. Y. Maistrenko, National Academy of Sciences of Ukraine, Institute of Mathematics and National Center for Medical and Biotechnical Research, Kiev, March 21–26.
47. ———, October 24–30.
48. ———, November 29 – December 5.
49. M.M. Malamud, Donetsk National University, Department of Mathematics, Ukraine, July 7–11.
50. D. Malioutov, Massachusetts Institute of Technology, Stochastic Systems Group, USA, November 6–14.
51. M. Malioutov, Northeastern University, Department of Mathematics, Boston, USA, July 1–9.
52. A. Manolescu, Reykjavik University, School of Science and Engineering, Iceland, June 1–20.
53. Ch. Meyer, Technische Universität Darmstadt, Graduate School of Computational Engineering, December 12–18.

54. M.D. Monteiro Marques, Universidade de Lisboa, Departamento de Matemática, Portugal, May 17–24.
55. A. Münch, University of Oxford, Oxford Center for Industrial and Applied Mathematics, Mathematical Institute, UK, January 24–27.
56. ———, May 5–11.
57. ———, June 21 – July 2.
58. ———, July 26 – August 20.
59. ———, December 6–10.
60. O. Muscato, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, July 30 – August 7.
61. R. Nickl, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, September 12–15.
62. F. Nier, Université de Rennes 1, Institut de Recherche Mathématique de Rennes (IRMAR), France, May 24–29.
63. ———, October 16 – November 13.
64. J. Novo, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Spain, November 1–5.
65. J. Outrata, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, November 1–30.
66. L. Paoli, Université de Saint-Etienne, Laboratoire de Mathématiques, France, January 5 – February 5.
67. ———, June 7–18.
68. V. Patilea, Institut National des Sciences Appliquées, Centre des Mathématiques, Rennes, France, June 13–19.
69. C. Patz, Robert Bosch GmbH, Stuttgart, October 27 – November 1.
70. J. Pfefferer, Universität der Bundeswehr München, Institut für Mathematik und Bauinformatik, Neubiberg, November 29 – December 3.
71. P. Philip, Universität München, Mathematisches Institut, February 22–26.
72. D. Rachinskii, University College Cork, Department of Applied Mathematics, Ireland, November 18–21.
73. J. Rademacher, Centrum voor Wiskunde & Informatica, Department Modelling, Analysis and Simulation, Amsterdam, The Netherlands, March 22–26.
74. J. Richet, École Normale Supérieure, Département Mathématique, Paris, France, May 1 – August 9.
75. R. Richter, Max-Plank-Institut Halbleiterlabor, München, August 23–26.
76. E. Rocca, Università degli Studi di Milano, Dipartimento di Matematica “Federigo Enriques”, Italy, October 18–27.
77. ———, November 15–19.
78. Th. Roche, Technische Universität München, Fakultät für Mathematik, November 22–26.
79. E. Roquain, Université Paris 6, Laboratoire de Probabilités et Modèles Aléatoires, France, June 7–11.
80. R. Rossi, Università di Brescia, Dipartimento di Matematica, Italy, April 19 – May 14.
81. A.H. Rotaru, Academy of Sciences of Moldova, Institute of Applied Physics, Chisinau, September 1–27.
82. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, January 25 – February 24.

83. ———, June 14 – July 13.
84. ———, November 24 – December 23.
85. G. Savaré, Università di Pavia, Dipartimento di Matematica, Italy, July 4–8.
86. O. Schenk, University of Basel, Department of Computer Science, Switzerland, March 21–26.
87. F. Schilder, Technical University of Denmark, Department of Mathematics, Kgs. Lyngby, December 16–21.
88. Ch. Schulz, Freie Universität Berlin, Fachbereich Mathematik, July 26 – September 3.
89. J. Sokołowski, Université de Nancy 1, Laboratoire de Mathématiques, Vandœuvre-lès-Nancy, France, April 26 – May 1.
90. F. Thein, Otto-von Guericke Universität Magedeburg, October 11 – December 17.
91. V. Topinsky, State University — Higher School of Economics, Moscow, Russia, February 14–20.
92. D. Turaev, Imperial College London, Department of Mathematics, UK, July 24 – August 13.
93. A. Vainchtein, University of Pittsburgh, Department of Mathematics, USA, December 13–19.
94. M. Yamamoto, University of Tokyo, Department of Mathematical Sciences, Japan, May 8–25.
95. ———, September 16 – October 4.
96. V. Zagrebnov, Université Aix-Marseille 2, Centre de Physique Théorique, Marseille, France, July 5–11.
97. ———, December 2–5.
98. H. Zähle, Universität des Saarlandes, Fachbereich Mathematik, Arbeitsgruppe Stochastik, November 1–4.
99. Ch. Zanini, Università degli Studi di Udine, Dipartimento di Matematica e Informatica, Italy, May 2–7.
100. S. Zelik, University of Surrey, Faculty of Engineering and Physical Sciences, Department of Mathematics, Guildford, UK, July 26 – August 20.
101. B. Zhang, Chinese Academy of Sciences, LSEC and Institute of Applied Mathematics, Beijing, Republic of China, July 19 – August 16.

A.12.2 Scholarship Holders

1. N. Berger, The Hebrew University of Jerusalem, Einstein Institute of Mathematics, Israel, Humboldt Research Fellowship, September 1, 2010 – July 31, 2011.
2. P. Friz, Technische Universität Berlin, Institut für Mathematik, WIAS, June 12, 2009 – June 11, 2014.
3. S. Ganesan, Otto-von-Guericke-Universität Magdeburg, Fakultät für Mathematik, Humboldt Research Fellowship, May 1, 2010 – April 30, 2012.

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. M. Liero, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 “Analysis, Numerics, and Optimization of Multiphase Problems”, doctoral candidate, December 1, 2008 – July 31, 2010.
3. 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, 2010.

4. 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.
5. L. Panizzi, Scuola Normale Superiore, Pisa, Italy, doctoral candidate, October 1, 2008 – March 5, 2010.
6. C. Patz, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, doctoral candidate, March 1, 2009 – April 30, 2011.
7. M. Roland, Universität des Saarlandes, Fachrichtung Mathematik, doctoral candidate, July 1, 2005 – May 19, 2010.
8. M. Salvi, Technische Universität Berlin, International Research Training Group GRK 1339: “Stochastic Models of Complex Systems and Their Applications”, doctoral candidate, April 1 – December 28.
9. 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.
10. 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.
11. A. Schnitzler, Technische Universität Berlin, International Research Training Group GRK 1339: “Stochastic Models of Complex Systems and Their Applications”, doctoral candidate, April 1 – December 31.
12. M. Thomas, Humboldt-Universität zu Berlin, Research Training Group GRK 1128 “Analysis, Numerics, and Optimization of Multiphase Problems”, doctoral candidate, January 1, 2007 – January 10, 2010.
13. W. Wang, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, doctoral candidate, October 1, 2009 – March 31, 2012.

A.13 Guest Talks

1. F. Abdenur, Pontifical Catholic University of Rio de Janeiro (PUC), Brazil, *Geometric mechanisms for robust transitivity*, February 2.
2. Th. Ackemann, University of Strathclyde, SUPA and Department of Physics, Glasgow, UK, *Semiconductor cavity soliton lasers based on frequency-selective feedback*, May 20.
3. St. Adams, University of Warwick, Mathematics Institute, Coventry, UK, *Probabilistic approaches to Bose–Einstein condensation*, September 1.
4. P. Alquier, Université Paris 7, Laboratoire de Probabilités et Modèles Aléatoires, France, *PAC-Bayesian bounds for sparse regression estimation with exponential weights*, December 1.
5. U. Assmann, Universität Duisburg-Essen, Fachbereich Mathematik, *Identification of an unknown parameter in the main part of an elliptic PDE*, September 28.
6. J.-Y. Audibert, Université Paris Est, École des Ponts ParisTech, Ingénierie Mathématiques et Informatique, France, *Risk bounds in linear regression through PAC-Bayesian truncation*, January 13.
7. H.-U. Balzer, St. Köhler, Humboldt-Universität zu Berlin, Institut für Agrar- und Stadtökologische Projekte (IASP), *Zeitreihenanalysen und experimentelle Erkenntnisse zur Darstellung biologischer Regelvorgänge*, May 31.
8. G.R. Barrenechea, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, *Residual local projection finite element methods*, August 26.
9. B. Basrak, University of Zagreb, Department of Mathematics, Croatia, *Regularly varying multivariate time series*, October 27.
10. M. Becker, Universität Leipzig, Mathematisches Institut, *Moments and distributions of the local times of a transient random walk on* Z^d, January 22.
11. N. Berger, The Hebrew University of Jerusalem, Einstein Institute of Mathematics, Israel, *A local CLT for random walk in random environment and applications*, November 3.
12. ———, *Spin-glasses on* Z^2 *— Many questions, very few answers*, November 26.
13. M. Biskup, University of California, Los Angeles, Department of Mathematics, USA, *Gibbs measures on permutations of the integers*, September 1.
14. G. Blöcher, Helmholtz-Zentrum Potsdam, Deutsches GeoForschungsZentrum, *Meshing and numerical solvers*, March 4.
15. N. Bochkina, University of Edinburgh, The School of Mathematics, UK, *Bayesian wavelet estimators: Optimality and a priori assumptions*, June 23.
16. A. Bovier, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Angewandte Mathematik, *Metastability in Ginzburg–Landau type SPDEs*, January 27.
17. O. Boyarkin, Universität Augsburg, Institut für Mathematik, *A positivity-preserving ALE finite element scheme for convection-diffusion equations in moving domains*, November 9.
18. J. Bradic, Princeton University, Department of Operations Research and Financial Engineering, Statistics Lab, USA, *Penalized composite quasi-likelihood for ultrahigh-dimensional variable selection*, July 7.
19. R. Brunsch, Leibniz-Institut für Agrartechnik Potsdam-Bornim (ATB), *Ansätze zur Verbesserung landwirtschaftlicher Produktionsverfahren durch Modellierung an der Schnittstelle zwischen Biologie und Technik*, May 31.
20. B. Bugert, Friedrich-Alexander-Universität Erlangen-Nürnberg, Lehrstuhl für Angewandte Mathematik II, *Cloaking for time-harmonic 3D Maxwell's equations*, May 5.

21. E. Burman, University of Sussex, Department of Mathematics, Brighton, UK, *Nitsche's method and unfitted FEM*, October 14.
22. C. Butucea, Université des Sciences et Technologies de Lille 1, Laboratoire Paul Painlevé, France, *Quantum statistics and U-operators*, November 24.
23. M. Cacace, Helmholtz-Zentrum Potsdam, Deutsches GeoForschungsZentrum, *Requirements for geosciences*, March 4.
24. A. Christmann, Universität Bayreuth, Fakultät für Mathematik, Physik und Informatik, *Some recent results on support vector machines*, May 5.
25. R. Čiegis, Vilnius Gediminas Technical University, Department of Mathematical Modeling, Lithuania, *Numerical solution of parabolic problems with nonlocal boundary conditions*, November 4.
26. R. Driben, Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, *Solitary wave propagation and supercontinuum generation in composites doped with silver nanoparticles*, April 15.
27. F. Durante, Freie Universität Bozen, Fakultät für Wirtschaftswissenschaften, Italy, *Tail dependence and copula*, April 28.
28. A. Ern, Université Paris-Est, Centre d'Enseignement et de Recherche en Mathématiques et Calcul Scientifique (CERMICS), Marne la Vallée, France, Matheon *Special Guest Lecture: Discontinuous Galerkin methods, Part I*, October 11.
29. ———, Matheon *Special Guest Lecture: Discontinuous Galerkin methods, Part II*, October 13.
30. ———, Matheon *Special Guest Lecture: Discontinuous Galerkin methods, Part III*, October 15.
31. ———, Matheon *Special Guest Lecture: Discontinuous Galerkin methods, Part IV*, October 20.
32. A. Faraj, Technische Universität Braunschweig, Institut für Analysis und Algebra, *Reduced model and simulations for the adiabatic evolution of quantum observables driven by 1D shape resonances*, November 10.
33. A. Fiaschi, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche, Pavia, Italy, *A Young-measure approach to a quasistatic-evolution problem for a phase-transition model*, May 19.
34. B. Fiedler, Freie Universität Berlin, Institut für Mathematik I, *Global attractors of Sturm type: Examples and counterexamples*, May 18.
35. M. Fila, Comenius University in Bratislava, Department of Applied Mathematics and Statistics, Slovak Republic, *Homoclinic and heteroclinic orbits for a semilinear parabolic equation*, June 8.
36. A. Fügenschuh, Konrad-Zuse-Zentrum für Informationstechnik, Berlin, *A data-mining linear programming model to predict material fatigue parameters & The Coolest Path Problem*, November 2.
37. F. Garwe, Institut für Photonische Technologien Jena (IPHT) e. V., *Wechselwirkung von Licht mit metallischen Nanopartikeln in dielektrischer Umgebung*, December 13.
38. J. Gatheral, New York University, Courant Institute of Mathematical Sciences, USA, *Random matrix theory and correlation estimation*, May 11.
39. M. Gerdts, Universität Würzburg, Institut für Mathematik, *Numerische Verfahren für gemischtganzzahlige Optimalsteuerungsprobleme*, August 24.
40. J. Giesselmann, Universität Stuttgart, Institut für Angewandte Analysis und Numerische Simulation, *Asymptotic analysis for Korteweg models*, February 2.
41. T. Girnyk, National Taras Shevchenko University, Mechanics and Mathematics Faculty, Kiev, Ukraine, *Twisted and multitwisted waves in a network of repulsive coupled oscillators*, March 24.

42. D. Glazkov, Yaroslavl Demidov State University, Department of Mathematics, Russia, *Qualitative analysis of one class of optoelectronic systems with singularly perturbed models*, September 28.

43. St. Grönneberg, University of Oslo, Department of Mathematics, Norway, *On the errors committed by sequences of estimator functionals*, January 26.

44. A. Gushchin, Steklov Mathematical Institute, Department of Probability Theory and Mathematical Statistics, *On superreplication prices in a general dynamic market model*, November 23.

45. L.G. Gyurko, University of Oxford, Mathematical Institute, *Cubature on Wiener space and the estimation of path dependent functions*, April 20.

46. R. Hable, Universität Bayreuth, Fakultät für Mathematik, Physik und Informatik, *Asymptotic normality of support vector machines*, November 9.

47. R. Haller-Dintelmann, Technische Universität Darmstadt, Fachbereich Mathematik, *The square root of divergence form operators with mixed boundary conditions*, September 29.

48. P.R. Hansen, Stanford University, Economics Department, Palo Alto, USA, *Realized GARCH: A complete model of returns and realized measures of volatility*, February 3.

49. J. Heiland, Technische Universität Berlin, Institut für Mathematik, *Control of drop size distributions in liquid/liquid dispersions*, September 2.

50. E. Hoarau, Agence Nationale pour la Gestion des Déchets Radioactifs, Direction Scientifique, Service Colis et Matériaux, Chatenay-Malabry, France, *Finite-volume simulation of carbon steel corrosion in a nuclear waste repository*, November 11.

51. A. Janssen, Heinrich-Heine-Universität, Mathematisches Institut, Düsseldorf, *Anwendungen der Le Cam Theorie in der Finanzmathematik*, January 20.

52. O. Kastner, Ruhr-Universität Bochum, Institut für Werkstoffe, *Microstructure formation and hysteresis in shape memory alloy*, April 26.

53. A. Khludnev, Russian Academy of Sciences, Lavrentyev Institute of Hydrodynamics, Novosibirsk, *Elastic bodies with thin rigid inclusions*, January 28.

54. D. Klingbeil, Bundesanstalt für Materialforschung und -prüfung Berlin (BAM), *Nicht-lokale Schädigungsmodelle bei großen Dehnraten — Modellbildung, Analyse der Gleichungen und auftretende Probleme*, December 13.

55. F. Klopp, Université Paris 13, Département de Mathématiques, Institut Galilée, France, *Spectral statistics for random operators in the localized regime*, January 20.

56. P. Knobloch, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, *Local projection stabilization for convection-diffusion-reaction equations*, August 12.

57. ———, *Stabilized finite element methods for convection-diffusion equations*, November 29.

58. M. Kraft, University of Cambridge, Department of Chemical Engineering, UK, *A moment and stochastic field method for turbulent reactive flow*, September 14.

59. P. Krejčí, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, *What happens when water freezes in an elastoplastic container?*, October 27.

60. ———, *Inversion of hysteresis operators*, November 23.

61. D. Kristensen, Columbia University, Economics Department, New York, USA, *Stochastic demand and revealed preference*, May 19.

62. A. Kulikovsky, Forschungszentrum Jülich GmbH, *Analytical modeling of fuel cells*, December 16.

63. Y. Latushkin, University of Missouri, Department of Mathematics, Columbia, USA, *Birman–Schwinger operators, Evans function and stability of wave solutions*, July 14.

64. H. Le-Minh, Humboldt-Universtität zu Berlin, Fachbereich Mathematik, *Saddle point model selection with application to multiple testing*, May 11.

65. E. Lieb, Princeton University, Department of Physics, USA, *Second thoughts on the second law of thermodynamics*, January 6.

66. M. Liero, Humbold-Universität zu Berlin, Institut für Mathematik, *The Allen–Cahn equation with dynamic boundary condition*, February 3.

67. R. Liptser, Tel Aviv University, Department of Electrical Engineering — Systems, *Modification of Beneš approach. New proof and applications*, June 22.

68. J. Liu, Southeast University, Department of Mathematics, Nanjing, Republic of China, *Numerical implementations of magnetic resonance electrical impedance tomography*, July 20.

69. M.M. Malamud, Donetsk National University, Department of Mathematics, Ukraine, *On the spectral theory of Schrödinger operators with point interactions*, July 9.

70. D. Malioutov, Massachusetts Institute of Technology, Stochastic Systems Group, USA, *Sparsity in signal processing, finance and machine learning*, November 10.

71. A. Manolescu, Reykjavik University, School of Science and Engineering, Iceland, *Time dependent transport, generalized master equation, and Coulomb interaction in quantum nanosystems*, June 9.

72. D. Matthes, Technische Universität Wien, Institut für Analysis und Scientific Computing, Austria, *A gradient flow approach to Cahn–Hillard and lubrication equations*, June 23.

73. Ch. Meyer, Technische Universität Darmstadt, Graduate School of Computational Engineering, *C-stationarity for optimal control of static plasticity*, December 14.

74. M.D. Monteiro Marques, Universidade de Lisboa, Departamento de Matemática, Portugal, *On sweeping processes and applications to dynamical and quasistatic problems*, May 19.

75. P. Mueller, University of Texas, MD Anderson Cancer Center, Houston, USA, *Bayesian approaches to multiple testing*, October 20.

76. J. Naumann, Humbold-Universität zu Berlin, Institut für Mathematik, *On weak solutions to model problems for turbulent flows*, February 17.

77. D. Naumov, Helmholtz-Zentrum Potsdam, Deutsches GeoForschungsZentrum, *Fluid flow in sandstones*, March 4.

78. St. Neukamm, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Derivation of a homogenized bending-torsion theory for inextensible rods from 3D elasticity*, December 15.

79. F. Nier, Université de Rennes 1, Institut de Recherche Mathématique de Rennes (IRMAR), France, *Adiabatic evolution of resonances in far-from-equilibrium systems*, October 27.

80. J. Novo, Universidad Autónoma de Madrid, Instituto de Ciencias Matemáticas, Spain, *Adaptive schemes for evolutionary convection dominated problems*, November 4.

81. A. Nowakowski, University of Łódź, Faculty of Mathematics and Computer Science, Poland, *Dynamic programming approach to structural optimization problem — Numerical algorithm*, December 7.

82. M. Ostermeyer, Innovative Berlin Laser GmbH (IBL), *Realizing excellent beam quality in high power solid state lasers — Search for a design tool*, October 25.

83. J. Outrata, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, *On the analysis of parametric equilibrium problems*, November 16.

84. L. Paoli, Université de Saint-Etienne, Laboratoire de Mathématiques, France, *A time-stepping scheme for multibody dynamics with unilateral constraints*, January 20.

85. L. Pastur, B.I.Verkin Institute for Low Temperature Physics & Engineering, Department of Theoretical Physics, Kharkov, Ukraine, *Limiting laws for the eigenvalue statistics of large random matrices*, May 26.

86. V. Patilea, Institut National des Sciences Appliquées, Centre des Mathématiques, Rennes, France, *Bandwidth-robust inference with conditional moment restrictions*, June 15.

87. P. Perlikowski, Technical University of Łodz, Division of Dynamics, Poland, *Dynamics in a ring of delayed coupled Stuart–Landau oscillators*, February 9.

88. J. Pfefferer, Universität der Bundeswehr München, Institut für Mathematik und Bauinformatik, Neubiberg, L^2 *error estimates on the boundary for the Neumann problem with application to optimal control*, November 30.

89. D. Picard, G. Kerkyacharian, Université Paris 7, Laboratoire de Probabilités et Modèles Aléatoires, France, *Well localized frames, representation of function spaces, and heat kernel estimates*, November 17.

90. A. Pimenov, University College Cork, Environmental Research Institute, Ireland, *Numerical study of dynamical regimes in passively mode-locked semiconductor laser*, September 28.

91. J. Piprek, NUSOD Institute LLC, Newark, USA, *GaN-based VCSELs: Simulation of internal device physics and analysis of performance limitations*, April 22.

92. D. Rachinskii, University College Cork, Department of Applied Mathematics, Ireland, *An injected mode locked laser*, November 18.

93. J. Rademacher, Centrum voor Wiskunde & Informatica, Department Modelling, Analysis and Simulation, Amsterdam, The Netherlands, *Riemann solvers and undercompressive shocks of convex FPU chains*, March 23.

94. J. Rang, Technische Universtät Braunschweig, Institut für Wissenschaftliches Rechnen, *Diagonally implicit Runge–Kutta methods and order reduction*, April 22.

95. L. Recke, Humboldt-Universität zu Berlin, Institut für Mathematik, *Nonresonant locking of self-pulsations under modulated optical injection*, June 3.

96. R. Richter, Max-Planck-Institut Halbleiterlabor, Technology, München, *Design and simulation of a silicon radiation detector for the Belle II experiment*, March 25.

97. S. Riecke, Ferdinand-Braun-Institut/PicoQuant GmbH, Berlin, *Mode competition in DFB lasers — Experiments and rate-equation simulation*, November 18.

98. F. Rindler, Oxford University, Mathematical Institute, UK, *Minimization problems in the space BD of functions of bounded deformation*, December 16.

99. K. Ritter, Technische Universität Darmstadt, Fachbereich Mathematik, *Multi-level algorithms for infinite-dimensional integration*, February 3.

100. E. Rocca, Università degli Studi di Milano, Dipartimento di Matematica "Federigo Enriques", Italy, *A diffuse interface model for two phase compressible fluids*, October 27.

101. ———, *On a non-isothermal model for nematic liquid crystals*, November 16.

102. Th. Roche, Technische Universität München, Fakultät für Mathematik, *Quasivariational sweeping processes on functions of bounded variation*, November 24.

103. R. Rossi, Università di Brescia, Dipartimento di Matematica, Italy, *Analysis of adhesive contact with thermal effects*, May 5.

104. A.H. Rotaru, Academy of Sciences of Moldova, Institute of Applied Physics, Chisinau, *Nonlinear effects of Bose-condensed phonons in biological systems*, September 22.

105. Ch. Rothe, Toulouse School of Economics, Research Group Econometrics and Statistics, France, *Analyzing counterfactual distributions*, June 30.

106. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, *Quasistatic plasticity with vanishing hardening*, February 10.

107. R. Samworth, University of Cambridge, Department of Pure Mathematics and Mathematical Statistics, UK, *Maximum likelihood estimation of a multidimensional log-concave density*, July 14.

108. G. Savaré, Università di Pavia, Dipartimento di Matematica, Italy, *The one-dimensional sticky particle system: An approach via optimal transport*, July 7.

109. O. Schenk, University of Basel, Department of Computer Science, Switzerland, *Linear algebra techniques in interior point methods for optimization*, March 25.

110. F. Schieweck, Otto-von-Guericke Universität Magdeburg, Institut für Analysis und Numerik, *A stable discontinuous Galerkin–Petrov time discretization of higher order*, March 18.

111. F. Schilder, Technical University of Denmark, Department of Mathematics, Kgs. Lyngby, *Continuation of constrained orbit segments: Algorithms and applications*, December 16.

112. S.A. Shapiro, Freie Universität Berlin, Fachbereich Geowissenschaften, *Fluid-induced seismicity and pore-pressure diffusion in rocks*, January 26.

113. J. Sieber, University of Portsmouth, Department of Mathematics, UK, *Dimension reduction for nonlinear periodic delay problems*, June 17.

114. D. Skoczowsky, Universität Potsdam, Institut für Physik und Astronomie, *Emission characteristics of broad area diode lasers in external cavities*, July 8.

115. J. Sokołowski, Université de Nancy 1, Laboratoire de Mathématiques, Vandœuvre-lès-Nancy, France, *Topological derivatives in shape optimization, an unified approach*, April 28.

116. S. Song, Humboldt-Universität zu Berlin, Institut für Statistik und Ökonometrie, *Flexible factor modelling in time and space*, April 14.

117. M. Spreemann, Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik (FBH), Berlin, *Finite Aperture Tapered Unstable Resonator Lasers (FATURLs): From idea to experimental verification*, February 4.

118. V. Springel, Heidelberger Institut für Theoretische Studien, *Tessellating the universe: Astrophysical fluid dynamics on a moving Voronoi mesh*, October 21.

119. M. Stingl, Universität Erlangen-Nürnberg, Institut für Angewandte Mathematik, *Material optimization: Towards a multi-scale approach*, January 21.

120. K. Strimmer, Universität Leipzig, Institut für Medizinische Informatik, Statistik und Epidemiologie, *High-dimensional feature selection by decorrelation: Application in genomics and proteomics*, June 16.

121. T. Stykel, Technische Universität Berlin, Institut für Mathematik, *Structure-preserving model reduction of second-order systems*, February 4.

122. M. Stynes, College of Science, Engineering and Food Science, School of Mathematical Sciences, Cork, Ireland, *A new finite element method for singularly perturbed reaction-diffusion problems*, November 29.

123. M. Sugiyama, H. Hachiya, Tokyo Institute of Technology, Department of Computer Science, Japan, *Density ratio estimation: A new versatile tool for machine learning*, September 14.

124. M. Timme, Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, *Spatio-temporal patterns in the brain: Neural networks with nonlinear dendrites*, January 26.

125. D. Turaev, Imperial College London, Department of Mathematics, UK, *Exponentially fast Fermi acceleration in slowly deformed billiards*, August 3.

126. A. Vainchtein, University of Pittsburgh, Department of Mathematics, USA, *Steady motion of a twinning dislocation*, December 14.

127. G. Wachsmuth, Technische Universität Chemnitz, Fakultät für Mathematik, *Regularity of displacement and stresses in linear and nonlinear elasticity with mixed boundary conditions*, April 14.

128. W. Welz, Technische Universität Berlin, Institut für Mathematik, *Tourenplanung in der Robotersteuerung*, June 1.

129. P. Winkert, Technische Universität Berlin, Institut für Mathematik, *Multiple solutions for nonlinear elliptic Neumann problems*, December 15.

130. M. Winkler, Universität Duisburg-Essen, Fakultät für Mathematik, *Irreversibly heading for balance? Some examples of colorful dynamics in simple diffusion processes*, June 8.

131. H.-J. Wünsche, Humboldt-Universität zu Berlin, Institut für Physik, *Modeling random semiconductor lasers: Scattered versus Fabry–Perot feedback*, June 24.

132. M. Yamamoto, University of Tokyo, Department of Mathematical Sciences, Japan, *Carleman estimates and the applications to inverse source problems for equations of fluid dynamics*, May 18.

133. ———, *Carleman estimate with second large parameter for second order hyperbolic operators in a Riemannian manifold and applications in thermoelasticity cases*, September 21.

134. Y. Yamaura, Nihon University, Department of Mathematics, Japan, *A scheme of construction of minimizing movement associated to the singular functional*, June 2.

135. I. Yousept, Technische Universität Berlin, Institut für Mathematik, *Optimal control of Maxwell's equations*, November 23.

136. V. Zagrebnov, Université Aix-Marseille 2, Centre de Physique Théorique, Marseille, France, *A partition-free approach to transient and steady-state charge currents*, July 7.

137. ———, *Trotter–Kato product formula: From Joint Institute for Nuclear Research to WIAS*, December 3.

138. H. Zähle, Universität des Saarlandes, Fachbereich Mathematik, *Limit theorems and robustness for tail-dependent statistical functionals*, November 2.

139. Ch. Zanini, Università degli Studi di Udine, Dipartimento di Matematica e Informatica, Italy, *A viscous damage model*, May 5.

140. S. Zelik, University of Surrey, Faculty of Engineering and Physical Sciences, Department of Mathematics, Guildford, UK, *Attractors and regularity for the Cahn–Hilliard equations with degenerate mobility*, August 10.

141. B. Zhang, Chinese Academy of Sciences, LSEC and Institute of Applied Mathematics, Beijing, Republic of China, *Uniqueness results for inverse scattering problems in periodic structures*, July 27.

142. St. Zunhammer, Humboldt-Universität zu Berlin, Institut für Mathematik, *Ein Modell für Risse in elasto-plastischen Materialien: Existenz einer globalen energetischen Lösung und Energiefreisetzungsrate*, June 9.

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/).

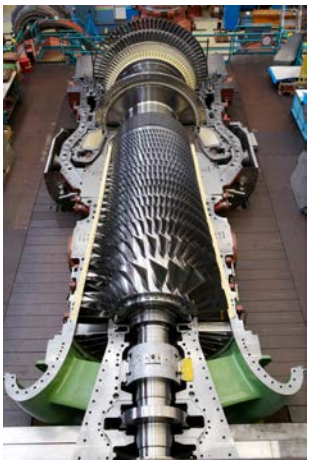
BOP (contact: J. Borchardt, phone: +49 30/20372-485, e-mail: juergen.borchardt@wias-berlin.de)

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



Assembly of an Alstom GT26 gas turbine at the Mannheim, Germany, facility

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 2010. Hence it makes use of the "Big Grid" spreadsheets and the new "PowerPivot".

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) and high angular resolution diffusion-weighted MR imaging (HARDI) data. It can be used to read DWI data, to estimate the diffusion tensor, for adaptive smoothing of DWIs, the estimation of orientation density functions, 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).

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.

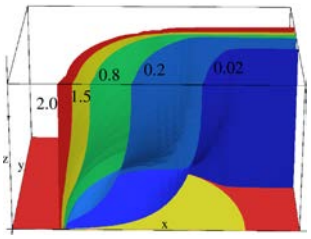
LDSL-tool combines models of different complexity, ranging from partial differential equation (PDE) to ordinary differential equation (ODE) systems. A mode analysis of the PDE system, a comparison of the different models, and a numerical bifurcation analysis of PDE systems are also possible.

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



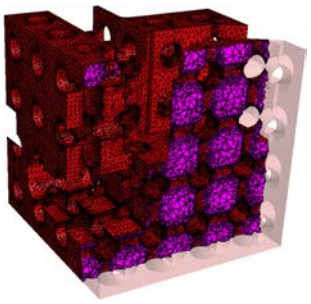
Concentration isosurfaces in a thin layer flow cell

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 and visualization tools for 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

- iterative solvers for linear and nonlinear systems of equations
- sparse matrix structures with preconditioners and direct solver interfaces
- dimension-independent simplex grid handling in one, two, and three space dimensions
- finite volume based solution of coupled parabolic reaction-diffusion-convection systems
- finite element based solution of variational equations (especially thermoelasticity) with goal-oriented error estimators
- optimization tool box
- parallelization on SMP architectures
- graphical output during computation using OpenGL
- scripting interface based on the language Lua
- graphical user interface based on the FLTK toolkit
- modular build system and package manager for the installation of third-party software used in the code

Please see also http://www.wias-berlin.de/software/pdelib.

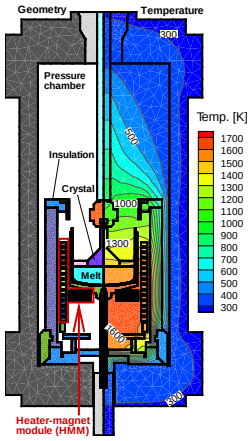


A cut view of a constrained Delaunay tetrahedral mesh of a complex 3D solid generated by TetGen

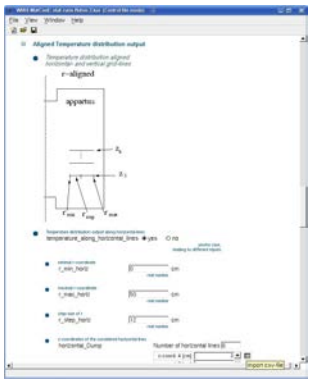
TetGen (contact: H. Si, phone: +49 30/20372-446, e-mail: hang.si@wias-berlin.de)

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.



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-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`.

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.