Leibniz Association

Weierstrass Institute for
Applied Analysis and Stochastics

Intelligent solutions for complex problems

Annual Research Report 2011

Cover figure: Collision of two pulses in an optical fiber in the frequency representation. Sudden changes in pulse parameters can be used to implement all-optical switching.

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ISSN 1437-7489
Berlin 2011

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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 2011. It gives a general overview of the scientific life, as well as an account of the scientific progress made in 2011. Following a more general introduction in part one, in its second part five selected scientific contributions, written for a broader public, highlight some results of outstanding importance. Finally, the third part presents the essential results of the research groups.

Prof. Dr. Jürgen Sprekels, Director

The main event in 2011 goes back to a decision taken by the General Assembly of the International Mathematical Union (IMU) in Bangalore (India) on August 16, 2010: WIAS was voted to become the host of the IMU Secretariat and thus the official address of IMU. This extraordinary event marked a real breakthrough for the institute's international reputation. The official opening of the IMU Secretariat was celebrated on February 1, when the two State Secretaries Dr. Georg Schütte (German Federal Ministry of Education and Research) and Dr. Knut Nevermann (Berlin Senate Department for Education, Science and Research) joined IMU President Prof. Dr. Ingrid Daubechies in the Ribbon Cutting Ceremony and the following Opening Ceremony. The eager staff of the IMU Secretariat, headed by the WIAS Deputy Director and newly elected IMU Treasurer Prof. Dr. Alexander Mielke, took up their duties, trying to serve mathematics and mathematicians all over the world. And it is quite noteworthy that already within the first year of its existence, the IMU Secretariat at WIAS has become a well-accepted meeting point of the worldwide mathematical community.

Another milestone for the future operation of the IMU Secretariat was the fact that the IMU Archive was moved from Helsinki to Berlin this year; the official opening of the Archive took place on November 10.

All this was only possible through 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 IMU Secrecariat 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 secretariat.

The main scientific highlight of 2011 was undoubtedly the "mega-grant" (approximately 3.4 million Euros) of the Russian government for Prof. Dr. Vladimir Spokoiny, the head of the Research Group *Stochastic Algorithms and Nonparametric Statistics*. Through the award of mega-grants, Russia wants to use the potential of internationally successful scientists and thereby strengthen its own research. The award winners have to use the money for the establishment of a research team at a college/university in Russia. This work is done parallel to the scientist's activities in the respective country.

Prof. Spokoiny is going to establish a research team with focus on "Predictive Modeling" in the field of information technologies at the renowned Moscow Institute of Physics and Technology. He is one of only four German mega-grant holders, which is an extraordinary recognition of his scientific standing.

Another highlight of 2011, which will strongly influence the institute's future efforts in the field of renewable energies, was the success of the head of the Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*, Prof. Dr. Wolfgang Dreyer, in the competition of Leibniz Association in the framework of the “Joint Initiative for Research and Innovation”. As a consequence, the Leibniz Group *Mathematical Models for Phase Transitions in Lithium Ion Batteries* will take up its work in 2012.

A further temporary structural change in the institute will become effective in the beginning of 2012. The institute’s Scientific Advisory Board recommended that the very successful Leibniz Group *Modeling of Damage Processes* should be continued for five years as a Young Scientists’ Group under the leadership of Dr. Dorothee Knees and Dr. Christiane Kraus.

Besides these important events of the year 2011, 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, 35 additional co-workers could be financed from grants.

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 2011: Dr. Ronny Loeffen (FG 6) moved to the University of Manchester for a position as a Senior Lecturer. Since the institute’s foundation in 1992, a total of 46 calls has been received by WIAS members, a truly remarkable output of which we are proud.

Eight international workshops organized by WIAS evidenced the institute’s reputation and its role as an attractive meeting place for international scientific exchange and cooperation. In addition, WIAS members (co-)organized numerous scientific meetings throughout the world, in particular, one at the Mathematisches Forschungsinstitut Oberwolfach.

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 2011, 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 2011 the joint operation of the DFG Research Center MATHEON “Mathematics for key technologies” located at the Technische Universität Berlin. The DFG funding of Matheon continues 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, Prof. 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 15 of its sub-projects. In turn, on Dec. 31, 2011, 13 scientific employees and several student assistants 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 February 2012

J. Sprekels

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1 WIAS in 2011

- 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.

The institute is committed to a policy of equal opportunity. It strives to increase the percentage of women within the scientific staff and, especially, in leading positions.

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 2011 organized into the departments for technical services, the Secretariat of the International Mathematical Union (IMU, see pages 50, 46), the seven scientific research groups, and one Leibniz group[1]:

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

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

The organization chart on the following page gives an overview of the organizational structure of WIAS in 2011.

1.2.2 Main Application Areas

The research at WIAS focused in 2011 on the following *main application areas*, in which the institute has an outstanding competence in modeling, analysis, stochastic treatment, and simulation:

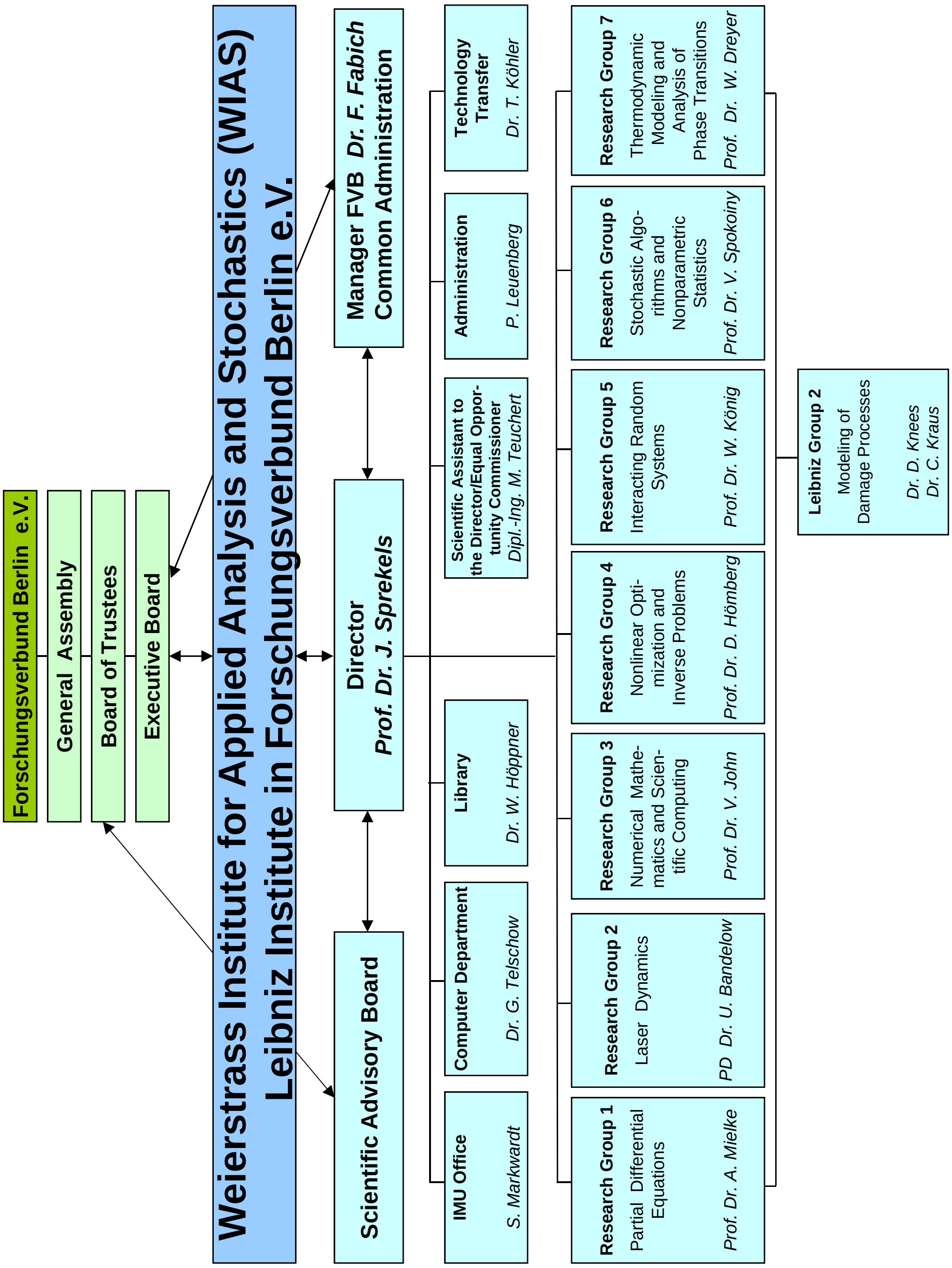
- **Nano- and optoelectronics**
- **Optimization and control of technological processes**
- **Phase transitions and multifunctional materials**
- **Flow and transport processes in continua**
- **Random phenomena in nature and economy**

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 Leibniz group 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, which necessitates a well-directed long-term *basic research in mathematics*.



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Prof. Dr. V. Spokoiny
Research Group 7
Thermodynamic Modeling and Analysis of Phase Transitions
Prof. Dr. W. Dreyer
Leibniz Group 2
Modeling of Damage Processes
Dr. D. Knees
Dr. C. Kraus

The table gives an overview of the main application areas to which the research and Leibniz groups contributed in 2011 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 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 2011 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)

– Photovoltaics (in RG 1 and RG 3)

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, analysis, and simulation of gas-solid and liquid-solid transitions, phase separation with thermomechanical diffusion (Stefan problems, phase field models, LSW theory, Becker–Döring models, in RG 7 and LG 2; and many-body systems, in RG 5)
- 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 2)
- Flow and mass exchange in porous media (in RG 3)
- 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)
- Mass transport in random media (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 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 processes in nonhomogeneous media (in RG 6 and RG 7)
- Branching processes in random media (in RG 5)
- Condensation phenomena in many-body systems (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 2011, having raised a total of 2.9 million euros, from which 35 additional researchers (+ 6.5 outside WIAS; Dec. 31, 2011) have been financed. In total in 2011, 28.2 per cent of the total budget of WIAS and 34.7 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].

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 2011, 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; Prof. 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 15 of its sub-projects. In turn, on Dec. 31, 2011, 13 scientists and several student assistants at WIAS were funded by MATHEON.

DFG Research Center MATHEON
Mathematics for key technologies

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.

Berlin Mathematical School

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

This international graduate college, which was operated jointly with ETH Zürich and University of Zurich, Switzerland, was another big success of the activities of Berlin’s mathematicians. The graduate college, whose funding period ran from July 2006 to March 2011, was located at the Technische Universität Berlin.

IRTG SMCP ZURICH BERLIN

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

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.

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).

DFG Collaborative Research Center (SFB) 910 *Control of Self-organizing Nonlinear Systems*

This center, which started in January 2011, involves groups at several institutes in Berlin, most of them working in physics. The sub-project A5 “Pattern formation in systems with multiple scales” (RG 1) focuses on the interaction between nonlinear effects relevant in pattern formation and the microstructures including the periodic settings as well as localized structures.

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 Dr. A. Münch/Prof. B. Wagner) and the third funding period (2008–2010, principal investigator Prof. B. Wagner) with the sub-project „Mathematical modeling, analysis, numerical simulation of thin films and droplets on rigid and viscoelastic substrates, emphasizing the role of slippage“ (RG 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 multiphase steel”.

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" (RG 3) within SPP 1276 runs in the third funding period that began in autumn 2011 after a positive evaluation of the program. Numerical methods for turbulent two-phase flows are developed and validated with experimental data, which are obtained from the scientist working in the project.

DFG Priority Program SPP 1506 *Transport Processes at Fluidic Interfaces*

This interdisciplinary priority program aims at a mathematically rigorous understanding of the behavior of complex multiphase flow problems with a focus on the local processes at interfaces. WIAS participates for the first funding period (2010–2013, principal investigator: Prof. B. Wagner) with the sub-project "Dynamics of viscous multi-layer systems with free boundaries" (RG 7).

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 international workshops in Dortmund, Bath (UK), and Munich in 2011. Research is devoted to a rigorous meso- and macroscopic analysis of large interacting systems with random input on microscopic scales.

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 2013).

DFG-CNRS Research Unit *Micro-Macro Modelling and Simulation of Liquid-Vapour Flows*

The research unit addresses cavitation problems, two phase flow in micro devices, cooling and boiling processes and breakup of liquid jets. WIAS contributes with a joint project of RG 7 and LG 2 on "Modeling and sharp interface limits of generalized Navier–Stokes–Korteweg systems".

EU FP7 Marie Curie Initial Training Network *PROPHET*

The Initial Training Network PROPHET (Postgraduate Research on Photonics as an Enabling Technology) aims to train young researchers in the field of photonics. This network started in the beginning of 2011 and is funded for 4 years by the EU 7th Framework Programme. The Weierstrass Institute (RG 2) is participating in the 1st Workpackage of the network: Photonics Enabling Communications Applications, which is mainly focused on the investigation of quantum dot mode-locked lasers.

ERC- Advanced Researcher Grant *AnaMultiScale — Analysis of multiscale systems driven by functionals*

The project ERC-2010-AdG no. 267802 is part of RG 1 and is funded by the European Research Council since April 2011 and lasts for 5 years. The research topics include the modeling and analysis of coupled physical systems such as elastic solids with internal variables, reaction-diffusion systems, and optoelectronic. The methods include variational techniques, gradient structures, Gamma convergence, and nonlinear PDE tools.

2 Scientific Highlights

- New Methods for the Valuation of Swing Options in Energy Markets
- Nonlocal Phase Separation and Damage Diffusion Processes
- Thermomechanical Modeling via Closed Systems Driven by Energy and Entropy Using GENERIC
- Nonlinear Optics in the Filamentation Regime
- Compatible Discretizations for Coupled Flow Problems

2.1 New Methods for the Valuation of Swing Options in Energy Markets

John Schoenmakers and Jianing Zhang

In recent years, the deregulation of the energy markets, in particular of the electricity and natural gas markets, has resulted in a higher uncertainty about the short- and intermediate-term development of commodity prices. Taking into account the complex structure of consumption and the restrictions on the storability of energy, the demand for financial instruments that allow for flexibility of the timing of delivery as well as of the amount of consumption has been on a constant rise. A prominent peculiarity that distinguishes the electricity market from other commodity markets is the fact that electricity cannot be stored.

One possibility to guarantee the market balance between electricity that is demanded and electricity that is provided is to trade on spot markets for electricity, e. g., the European Energy Exchange (EEX) based in Leipzig, Germany. During particular time slots, one or several packages of electricity can be traded at the price quoted on the spot market. However, these prices are typically governed by a highly oscillatory dynamic with the tendency to exhibit distinctive price peaks, intraday and over weeks and months. Hence, from the viewpoint of risk management, features that incorporate protection against price risks are called for. In this respect, swing options emerged that provide their owners with the right to repeatedly buy or sell packages of electricity subject to daily as well as periodic constraints. The number of packages that an owner can buy or sell is generally fixed in advance. Swing options thus equip their owners with flexibility of delivery and risk protection in a market characterized by spiking price behavior.

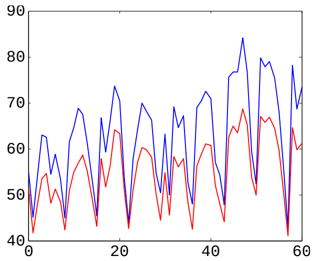

Fig. 1: *Base and peak spot prices Nov.–Dec. 2011*

Due to the typical complexity of the structure of a swing option, simulation-based methods for the numerical evaluation of such an option are most suited for the problem. Historically, simulation-based methods for the pricing of options with flexible exercise dates were first developed for American options (i. e., swing options with a single exercise right). In particular, the regression-based approach proposed in [2] has been considered a breakthrough in the late nineties. In general, the developed simulation methods provide lower bounds for option prices by constructing an approximation to the optimal exercise time via regression on a certain set of basis functions. As such, these approaches are termed *primal* and they provide a tool to bound the price from below. Shortly thereafter, the next breakthrough was provided by a *dual* representation [4], which expresses the option price as an infimum of an expectation over a set of martingales. By its very nature, this dual method bounds the price of an American option from above. Until recently, dual methods for more realistically structured swing options, for example, options that allow for volume constraints and refraction periods simultaneously, were, however, not available; cf. [3]. The study of dual valuation of standard multiple exercise options has proceeded in the Research Group *Stochastic Algorithms and Nonparametric Statistics* by developing a new dual martingale representation [5]. The latter approach was recently extended to a dual representation for far more general exercise profiles that cover swing options involving both volume constraints and refraction periods [1].

Dual representation for general multiple stopping problems

Let us consider a stylized swing contract that equips the owner with L exercise rights to buy at most one package of electricity over a period of T days at a fixed price $K > 0$. Once s/he has exercised a single right, s/he must wait for at least the next day until s/he is allowed to exercise again. The so-induced cashflow is given by

$$Z_j := \max\{0, S_j - K\} = (S_j - K)^+,$$

where S_j denotes the price of electricity on the j-th day. This means that if the owner decides to make use of one of his or her exercise rights, s/he does it when the price S_j is above the strike price K, thus enabling her to come off cheaper by saving the difference $S_j - K$. So, the strike price $K > 0$ is to be interpreted as the protection level of the owner against high prices. Now, the contract value at the issuing date takes into account all possible exercise strategies and is thus given by the maximized expected reward

$$V_0 := \sup_{0 \le \tau^1 < \ldots < \tau^L \le T} \mathbb{E} \sum_{k=1}^{L} Z_{\tau^k}.$$

In practice, the most common features of swing contracts are *volume constraints* and *refraction periods*. Volume constraints specify the maximal amount of electricity that can be bought on a single trading date. Refraction periods specify the minimal waiting time that must elapse before the owner can make use of his or her next right, after a swing right has been used.

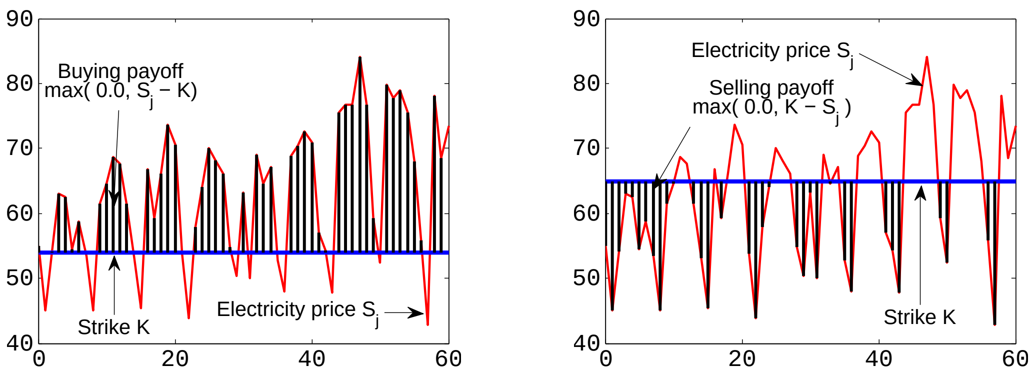

Fig. 2: *Left: Possible cashflows for buying electricity. Right: Possible cashflows for selling electricity.*

The mathematical formulation of a general multiple stopping problem starts with a given set of discrete time points $i = 0, \ldots, T$ with $T \in \mathbb{N}$ and an $(\mathcal{F}_i)$-filtered probability space. Now given $L \le T$ exercise rights, a cashflow is defined as a mapping $X : \{0, \ldots, T\}^L \times \Omega \to \mathbb{R}$, which satisfies for all $0 \le i_1 \le \cdots \le i_L \le T$,

$$X_{i_1,\ldots,i_L} \text{ is } \mathcal{F}_{i_L}\text{-measurable and } \mathbb{E}\left|X_{i_1,\ldots,i_L}\right| < \infty.$$

The *multiple stopping problem* is now constituted by

$$Y_i^{*,L} := \sup_{i \le \tau^1 \le \cdots \le \tau^L} \mathbb{E}_{\mathcal{F}_i} X_{\tau^1,\ldots,\tau^L},$$

where the (essential) supremum runs over a family of ordered stopping times $\tau^k, 1 \leq k \leq L$. One interprets the stopping times τ^k as the exercise times for pocketing L times the cashflow X, interspersed on $i, \dots, T$, and $Y_i^{*,L}$ as the value of L rights at time i if they are exercised optimally. Hence, today's price for having the flexibility to exercise L rights is equal to $Y_0^{*,L}$.

The theoretical backbone of approaching the price from above is provided by the following *dual* characterization of $Y_i^{*,L}$ in terms of so-called *martingales*, an important class of stochastic processes that are intimately linked to the concept of a fair game and to the no-arbitrage notion in financial modeling.

Theorem 1 (Bender, Schoenmakers and Zhang [1]):

(i) For any $0 \leq i \leq T$ and any set of martingales $\left(M_r^{L-k+1,j_1,\dots,j_{k-1}}\right)_{r \geq j_{k-1}}$, where $1 \leq k \leq L$ and $i =: j_0 \leq j_1 \leq \cdots \leq j_{k-1}$,

$$Y_i^{*,L} \leq \mathbb{E}_{\mathcal{F}_i} \max_{i \leq j_1 \leq \cdots \leq j_L} \left(X_{j_1,\dots,j_L} + \sum_{k=1}^{L} \left(M_{j_{k-1}}^{L-k+1,j_1,\dots,j_{k-1}} - M_{j_k}^{L-k+1,j_1,\dots,j_{k-1}} \right) \right).$$

(ii) For $0 \leq i \leq T$

$$Y_i^{*,L} = \max_{i \leq j_1 \leq \cdots \leq j_L} \left(X_{j_1,\dots,j_L} + \sum_{k=1}^{L} \left(M_{j_{k-1}}^{*L-k+1,j_1,\dots,j_{k-1}} - M_{j_k}^{*L-k+1,j_1,\dots,j_{k-1}} \right) \right),$$

where for $1 \leq k \leq L$, and $i =: j_0 \leq j_1 \leq \cdots \leq j_{k-1}$, $\left(M_r^{*L-k+1,j_1,\dots,j_{k-1}}\right)_{r \geq j_{k-1}}$ is the so-called *Doob martingale* of

$$Y_r^{*L-k+1,j_1,\dots,j_{k-1}} = \sup_{\tau \geq r} \mathbb{E}_{\mathcal{F}_r} Y_\tau^{*L-k,j_1,\dots,j_{k-1},\tau}, \quad r \geq j_{k-1}.$$

Roughly speaking, the first part states that the true price $Y_i^{*,L}$ can be approximated from above by assigning to each (remaining) exercise right a martingale $M^{L-k+1,j_1,\dots,j_{k-1}}$. The second part states that if one chooses the Doob martingales of the remaining rights as approximating family of martingales, conditional on having exercised the first $k-1$ rights at $j_1, \dots, j_{k-1}$, then one recovers exactly the price of the entire multiple exercise option. This result provides an abstract framework, which easily allows to model swing options under volume constraints and refraction periods. However, it should be stressed that the above dual representation relies on typically huge families of martingales $M_r^{L-k+1,j_1,\dots,j_{k-1}}$ parameterized via the $(k-1)$-tuples $(j_1, \dots, j_{k-1}), k = 1, \dots, L$.

Modeling volume constraints and refraction periods

Based on Theorem 1, we now turn towards the modeling of swing options with a twofold view: making the dual representation implementable on the one hand and allowing the cashflow to incorporate volume constraints and refraction periods on the other hand. To this end, let us consider a nonnegative process Z_j. The multiple stopping problem that we have in mind is to optimally exercise this cashflow under constraints on the set of admissible stopping times due to refraction periods and volume constraints. We first consider an adapted volume constraint process υ with values in $\{1,...,L\}$ such that $1 \le \upsilon_t \le L$ is the maximum number of rights that one may exercise at t. In order to formalize this constraint, we introduce for $p \ge 1$ the mapping $\mathcal{E}_p$ acting on a non-decreasing p-tuple $(j_1,\dots,j_p)$ by $\mathcal{E}_p(j_1,...,j_p) := \#\{r : 1 \le r \le p,\ j_r = j_p\}$. Hence, $\mathcal{E}_p$ denotes the number of rights exercised at j_p in the non-decreasing chain $0 \le j_1 \le \cdots \le j_p \le T$. Obviously, an ordered chain of stopping times $\tau^1 \le \cdots \le \tau^L$ satisfies the volume constraint if and only if $\mathcal{E}_p(\tau^1,...,\tau^p) \le \upsilon_{\tau^p}$ for every $p = 1,\dots,L$. The second constraint is the refraction period that specifies the minimal waiting time between two exercises at different times. We admit random refraction periods, i. e., at each time i, $0 \le i \le T$, we fix a stopping time ρ^i taking values in $\{i+1,...,T\}$. If at least one right is exercised at time i, then the refraction period constraint imposes that the next right must either be exercised at the same time (if consistent with the volume constraint) or otherwise no earlier than ρ^i. A standard case is $\rho^i = (i+\delta)\wedge T$, where $1 \le \delta \le T$ is deterministic. Both constraints can be summarized by the binary $\mathcal{F}_{j_p}$-measurable random variable

$$\mathcal{C}_p(j_1,...,j_p) := \begin{cases} 1, & \forall_{1\le l\le p} : \mathcal{E}_l(j_1,...,j_l) \le \upsilon_{j_l} \text{ and } \forall_{1\le l\le p} : j_l > j_{l-1} \Longrightarrow j_l \ge \rho^{j_{l-1}}, \\ 0, & \text{else,} \end{cases}$$

which is equal to 1 if and only if the constraints are satisfied when exercising at the p times $j_1 \le \cdots \le j_p$. By setting

$$X_{j_1,\dots,j_L} = \begin{cases} \sum_{k=1}^{L} Z_{j_k}, & \text{if } \mathcal{C}_L(j_1,,...,j_L) = 1, \\ -N, & \text{else,} \end{cases}$$

we have recast the swing contract under volume constraints and refraction periods into the framework of Theorem 1.[1]

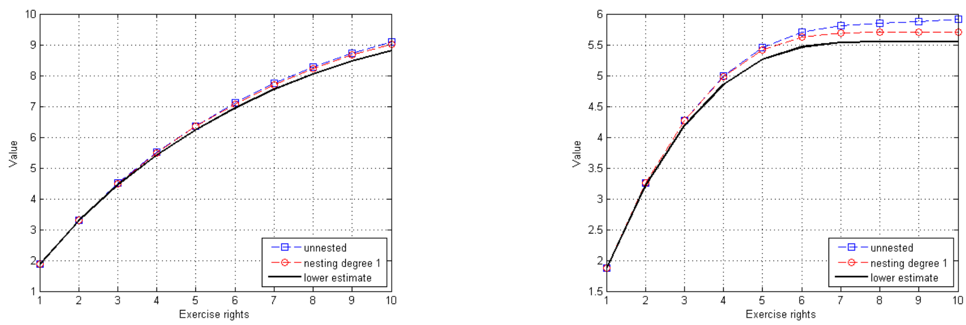

Fig. 3: *Left: Off-peak swing option with refraction $\delta = 2$. Right: Off-peak swing option with refraction $\delta = 10$.*

Constructing price intervals for swing options

Based on the theoretical framework sketched above, we have developed in [1] a hands-on numerical recipe to bound swing option prices from below and from above. As an example, we here

[1] The term $-N$ is to be interpreted as a penalty fee for violating the imposed constraints.

present the pricing of an *off-peak* swing option that allows to buy at most one package of electricity on weekdays and at most two packages on weekends. The trading window length is two months. Once exercise rights have been used at a particular day, the owner has to wait the refraction period $\delta \in \mathbb{N}$ days until s/he is allowed to buy electricity again. Figure 3 depicts lower and upper bounds for the swing option price under different refraction periods. The blue and red lines indicate upper bounds arising from variations of the dual representation from Theorem 1. We underline that since existing results from the literature are not able to deal with volume constraints and refraction periods simultaneously, this numerical implementation is a novelty and marks a completion of the literature.

δ	L	95% confidence interval	L	95% confidence interval
1	8	[9.59318, 9.62507]	10	[11.0332, 11.0677]
4	8	[7.99887, 8.06551]	10	[8.57102, 8.64178]
8	8	[6.17596, 6.23403]	10	[6.19445, 6.2513]
10	8	[5.54107, 5.59089]	10	[5.54107, 5.59089]

Table 1: *Confidence intervals for the price of the off-peak swing options with* 8 *and* 10 *rights*

Table 1 depicts 95% confidence intervals for the price of the off-peak swing option. This interval covers the true price with a probability of 95% and arises from computing lower and upper bounds for the price. Note that the relative length of the intervals is altogether below 1%, emphasizing that our numerical method produces tight bounds. Moreover, the method is also robust towards pathological contract design. If one considers the last line of Table 1, the confidence intervals for $L = 8$ and $L = 10$ rights are identical. The reason for this fact is that adding two additional rights to a swing contract with $L = 8$ rights under the refraction period $\delta = 10$ is useless: the $L = 8$ rights cannot be exhausted optimally in two months, having superfluous rights for which there is not enough time to exercise them. Thus, the price of the contract involving 8 exercise rights must be equal to the contract involving 10 rights.

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2.2 Nonlocal Phase Separation and Damage Diffusion Processes

Jens A. Griepentrog

Many interesting drift-diffusion processes in physics take place in a closed system with interacting particles of different type occupying a spatial domain. Within the DFG Research Center MATHEON project C32, we are interested in the *modeling of phase separation and damage processes in alloys* on a mesoscopic scale. It is well known that materials that enable the functionality of technical products change their microstructure over time. For instance, the complete failure of electronic devices often results from phase separation, agglomeration of particles of the same type, or voids and micro-cracks in solder joints; see Figures 1 and 2.

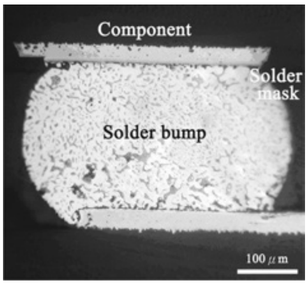

Fig. 1: *Optical micrograph of a typical solder joint, see [1, Figure 1]; accumulation of phases and coarsening*

Description of the physical phenomenon

Regarding an alloy as a multi-component mixture of (metallic) particles, all of the configurational changes are the result of processes that try to minimize the free energy of the whole ensemble. This free energy contains the sum of the binding energies between the particles with respect to their type and their distances. The mesoscopic scale of our model is larger than the single particle picture of quantum mechanics but smaller than the continuum mechanical limit: The averaged long-range interaction forces are explicitly described by attractive interaction potentials for particles of the same type. These forces lead to phase separation and coarsening phenomena. On the other hand, the short-range repelling forces are accounted for using the logarithmic distribution function of Fermi statistics reflecting the exclusion principle for particles with Fermi-type behavior to be explained under the next subsection. These forces are responsible for the diffusion process that enters in competition with phase separation. We incorporate damage processes by considering the diffusion of so-called *voids* or *vacancies*, being nothing but some special type of *noninteracting* particles of the multi-component system.

In the following, we give a brief summary of the model, and we illustrate the connection between its analytical and numerical stability properties by numerical simulations.

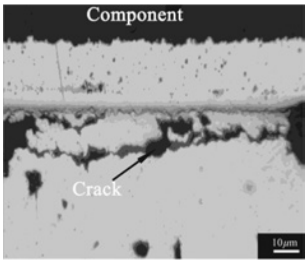

Fig. 2: *Optical micrograph of the crack in a failed solder joint, see [1, Figure 7], induced by thermal stress*

The model equations

The justification of our model relies on statistical mechanics: We assume that particles of different type jump around on a given microscopically scaled lattice following a stochastic exchange process. Note that voids or vacancies are admissible types of particles, too. Exactly one particle sits on each lattice site (exclusion principle). Two particles of type i and $\ell \in \{0, 1, \ldots, m\}$ change their sites x and y with a certain probability $p_{i\ell}(x, y)$, due to *diffusion* and *interaction*; see Figure 3. This process is symmetric, reversible, and translation invariant. That means that $p_{i\ell}(x, y) = p_{i\ell}(y, x) = p_{\ell i}(x, y)$ and $p_{i\ell}(x + z, y + z) = p_{i\ell}(x, y)$. Moreover, it tries to minimize the *free energy* of the particle ensemble.

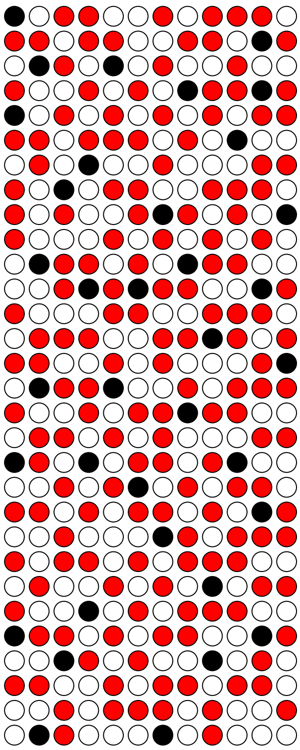

Fig. 3: *Particles of different type in a microscopically scaled lattice*

To carry over these properties from the discrete microscopic scale to the continuous mesoscopic level, statistical mechanics uses the hydrodynamical limit process: The number of particles in the lattice tends to infinity. As the result, the state of the mesoscopic ensemble is described by *densities* of particles occupying a spatial domain $\Omega \subset \mathbb{R}^n$. In [2], it was shown that this limit process leads to a system of $m+1$ conservation laws:

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

with scaled *mass densities* $u_0, \dots, u_m$, *initial values* $u_0^0, \dots, u_m^0$, and *current densities* $j_0, \dots, j_m$. Due to the exclusion principle, these densities are normalized, and they sum up to unity pointwise. Moreover, the closedness of the system enforces that the sum of all current densities vanishes:

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

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

Local minimizers of the *free energy functional* F under the constraint of mass conservation are supposed to be physically relevant equilibrium distributions $u^* = (u_1^*, \dots, u_m^*)$ of the multi-component system, and more generally, steady states of the energy-driven evolution system. Correspondingly, they can be found as solutions (u^*, λ^*) of the Euler–Lagrange equation $DF(u^*) = \lambda^*$, where $\lambda^* \in \mathbb{R}^m$ denote Lagrange multipliers. We define the free energy $F(u) = \Phi(u) + \Psi(u)$ of the distribution u as the sum of the strongly convex *chemical energy* or *segmentational entropy*

$$\Phi(u) = \int_\Omega \varphi(u(x))\,dx, \quad \varphi(u) = \sum_{i=0}^m u_i \log(u_i), \tag{2}$$

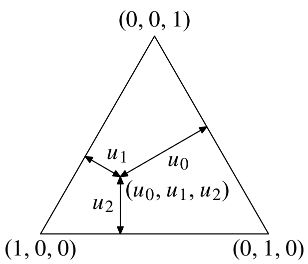

Fig. 4: *Ternary simplex with barycentric coordinates*

and of the *potential energy* $\Psi(u) = \Psi_{\text{int}}(u) + \Psi_{\text{ext}}(u)$. The latter is split into the *nonlocal energy*

$$\Psi_{\text{int}}(u) = \frac{1}{2}\int_\Omega \sum_{i=0}^m (Ku)_i(x)\,u_i(x)\,dx, \quad (Ku)_i(x) = \int_\Omega \sum_{\ell=0}^m k_{i\ell}(x,y)\,u_\ell(y)\,dy \tag{3}$$

of *self-interaction* and some part representing the *potential energy*, due to *external forces*,

$$\Psi_{\text{ext}}(u) = \int_\Omega \sum_{i=0}^m \psi_i(x)\,u_i(x)\,dx\,. \tag{4}$$

As mentioned above, the logarithmic potential φ in (2) reflects the Fermi-type behavior of the particles. It prevents the densities u_i to come too close to the boundary of the range $[0,1]$. This entropic part alone would prefer uniform distributions. To control the behavior of nonlocal interaction between particles of type i, $\ell \in \{0, \dots, m\}$, we use symmetric matrix kernels $(k_{i\ell})$, which ensure, for instance, that particles of the same type attract and particles of different type repel each other. This interaction leads to the desired phase separation. In Figure 5, an energy landscape for a ternary system of uniform distributions is plotted. Here, we have used barycentric coordinates;

see Figure 4. A cut along the baseline of the simplex leads to the typical double-well structure of the free energy for binary systems; see Figure 6. With the help of potentials ψ_i, we can apply external volume or boundary forces to the particles.

For the sake of numerical simplicity, according to (3), we define $(Ku)_i$ as the solution to the elliptic Neumann boundary value problem

$$-\nabla\cdot r^2\nabla(Ku)_i+(Ku)_i=\sum_{\ell=0}^{m}\sigma_{i\ell}u_\ell \quad \text{in } \Omega, \quad \nu\cdot r^2\nabla(Ku)_i=0 \quad \text{on } \partial\Omega. \tag{5}$$

Green's function to the corresponding elliptic operator is a radially decreasing kernel, which decays rapidly outside a ball of radius $r>0$. Hence, using the above setting, we prescribe effective ranges $r>0$ and intensities $\sigma_{i\ell}\in\mathbb{R}$ of interaction forces between particles of type i and ℓ. The cases $\sigma_{i\ell}>0$, $\sigma_{i\ell}<0$, $\sigma_{i\ell}=0$ represent repulsive interaction, attractive interaction, and no interaction, respectively. According to (4), we consider potentials ψ_i of effective range $\rho>0$ as solutions to elliptic problems

$$-\nabla\cdot\rho^2\nabla\psi_i+\psi_i=g_i \quad \text{in } \Omega, \quad \nu\cdot\rho^2\nabla\psi_i=h_i \quad \text{on } \partial\Omega, \tag{6}$$

where g_i and h_i are stationary or time-dependent external volume and boundary forces.

In view of the fact that the Lagrange multipliers λ_i^* should be constant, one assumes their antigradients to be driving forces towards equilibrium. This assumption leads to the evolution system (1)–(4) with current densities $j_i=-\sum_{\ell=1}^{m}a_{i\ell}(u)\nabla\lambda_\ell$, potentials $\lambda_\ell=D_\ell F(u)$, and positive semidefinite *mobility* matrices $(a_{i\ell})$. If all of the particles have the same diffusion coefficients, then the hydrodynamical limit process yields mobilities $a(u)$ that are given by the inverse Hessian $(D^2\Phi(u))^{-1}=(\delta_{i\ell}u_\ell-u_iu_\ell)$; see [2].

In [3], we have shown unique solvability, regularity properties, and uniform positivity of solutions to the evolution system (1)–(4). Moreover, for stationary external forces the solution converges asymptotically to a solution (u^*,λ^*) of the Euler–Lagrange equation

$$\lambda^*=D\Phi(u^*)+D\Psi(u^*), \qquad \int_\Omega u^*(x)\,dx=\int_\Omega u^0(x)\,dx.$$

The free energy decreases monotonically along the trajectory to the corresponding limit $F(u^*)$.

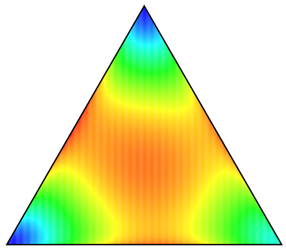

Fig. 5: *Energy diagram for a ternary system: Increasing energy from blue (separated phases) to red (mixed configurations) regions*

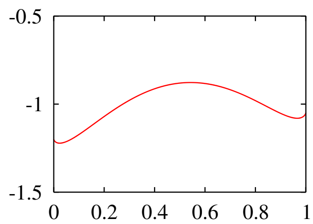

Fig. 6: *Cut along the baseline of the simplex in Figure 5 shows double-well structure*

Numerical examples

All of the above-mentioned properties of the continuous evolution system carry over to the dissipative discretization scheme used for our simulations; see [4]. It combines a Crank–Nicholson-type discretization in time with a Voronoi finite volume scheme on boundary-conforming Delaunay meshes in space. Figures 7 and 8 show numerical results for three-component phase separation processes in a square. The time series of evolutionary states follows equidistant points on a logarithmic scale. In both cases, the initial value is the same randomly chosen distribution of 10 % black ($i=0$), 45 % red ($i=1$), and 45 % white ($i=2$) particles.

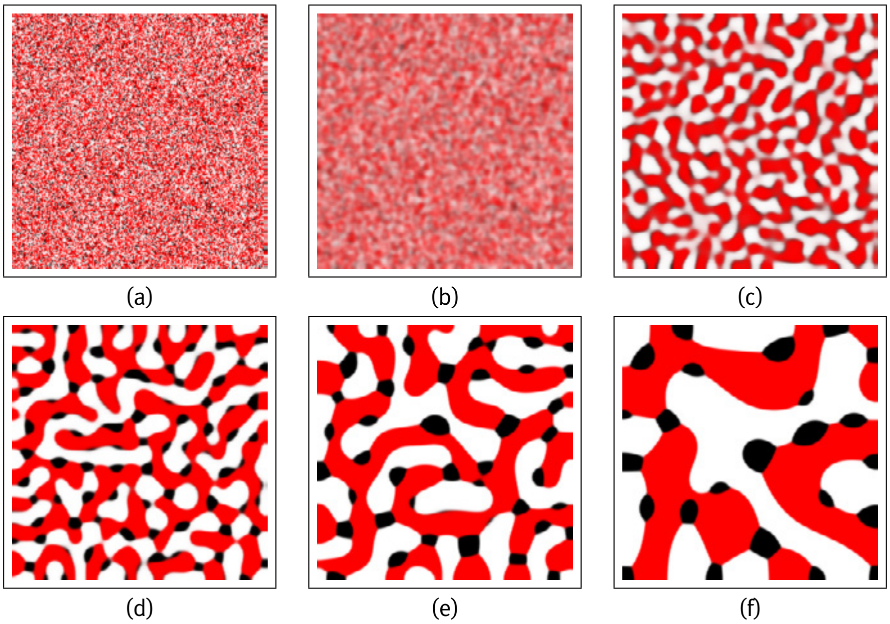

Fig. 7: *Phase separation process in a ternary system with a spatial discretization of 256 by 256 pixels. (a) Initial value. (b) Diffusion of particles. (c) Agglomeration and graining. (d) Fully separated phases. (e) Coarsening of phases. (f) Occurence of meta-stable states*

Phase separation in ternary systems. Figure 7 shows phase separation with uniform interaction intensities $\sigma_{ii} = -\sigma < 0$ (attraction) and $\sigma_{i\ell} = \sigma > 0$ (repulsion) for i, $\ell \in \{0, 1, 2\}$ with $i \neq \ell$ according to (5) and without external forces. This models the phase separation in an *incompressible* body consisting of a ternary system of equally treated components.

After initial diffusion, the particles start to agglomerate and to grain until they reach fully separated states. We observe triple points with typical angles of 120 degrees between the phases. Going on further, we see coarsening of phases and metastable states still being far from equilibrium.

Phase separation in binary systems with damage diffusion. The evolution of the system changes in Figure 8, where the (black) vacancies neither interact with themselves nor with red or white particles; we have modified $\sigma_{i\ell} = 0$ for $i = 0$, $\ell \in \{0, 1, 2\}$ in the above setting. Here, we describe the phase separation of red and white particles in a *compressible* body, which has 90 per cent of the unit density. The rest is filled up with vacancies. We have further modified the regime by applying stationary external forces at three boundary parts. The upper part, the lower half of the left, and the second quarter of the right part are loaded equally to press the red and white particles inwards. According to (6), we have set $h_0 = 0$, $h_1 \neq 0$ and $h_2 \neq 0$.

During the evolution, after initial diffusion, both the red and white components show agglomeration, graining, and slight denting at the pressure zones. Red and white particles reach the state of full separation and compression. They leave room for the vacancies to concentrate as damage channels at the interfaces between red and white phases, which show strong resistance, obstructing inward pressure. Further coarsening and hardening of phases leads to the thickening of damage channels and significant denting at the pressure zones. After that we arrive at metastable states, still being far from equilibrium.

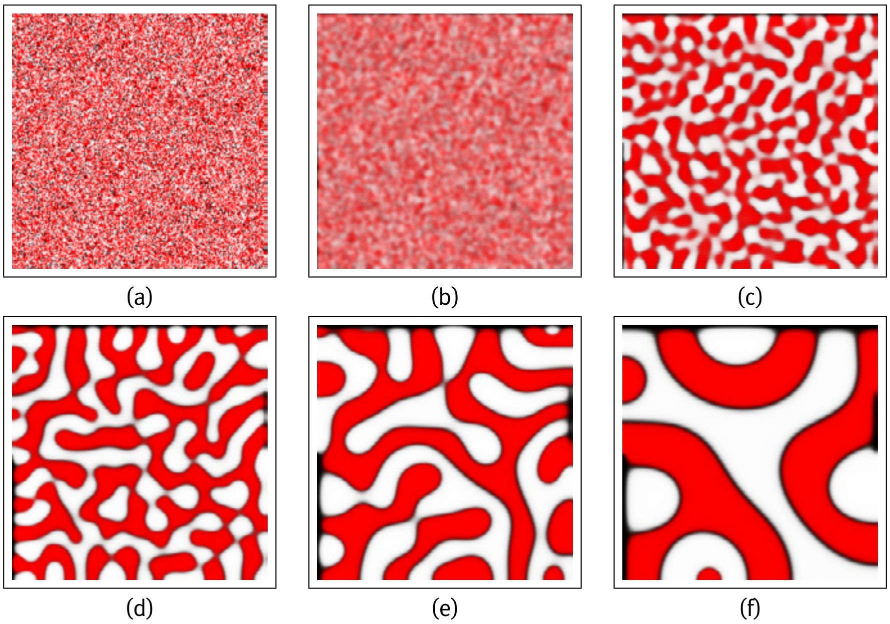

Fig. 8: *Phase separation process in a binary system with inward pressure. (a) Initial value. (b) Diffusion of particles. (c) Agglomeration, graining, and slight denting at the pressure zones. (d) Fully separated phases; vacancies concentrated at interfaces between the phases; (e) Coarsening and hardening of phases; thickening of damage channels; (f) Occurence of metastable states; concentration of damage channels near the pressure zones.*

Discussion and further problems

The mesoscopic scale of our nonlocal model is smaller than that of the local phase separation and damage models typically used in continuum mechanics. These models can be derived from ours by Taylor expansion under the assumption of small density deviations. Moreover, all the densities including that of the vacancies are conserved quantities.

In the future, we want to prove rigorously the above-mentioned unique solvability, regularity properties, and uniform positivity of solutions to our dissipative discretization scheme. Our second aim is the generalization to a (strongly coupled) nonisothermal model of phase separation, which incorporates an additional energy balance equation for the energy current density.

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2.3 Thermomechanical Modeling via Closed Systems Driven by Energy and Entropy Using GENERIC

Alexander Mielke and Marita Thomas

Fig. 1: *A flying ball can be modeled as a mass point using Newton's laws of motion*

Introduction. The traditional way of thermomechanical modeling of physical and chemical processes is based on the interplay of *universal balance laws* and the particular *constitutive laws* for the system under consideration. Here, we propose an alternative way of modeling that is more adapted to the underlying mathematical structures and tools. The general evolution of a system will be described as the sum of a reversible part, a Hamiltonian system driven by the energy, and an irreversible part, a gradient system driven by the entropy. The proper coupling is done in the framework of GENERIC, which is an acronym for General Equation for Non-Equilibrium Reversible-Irreversible Coupling; see [2].

A brief historical review

In order to get to know the most important ideas in history leading to GENERIC, let us start by throwing a ball; cf. Figure 1. Modeling it as a mass point or a rigid body, we can describe its motion using Newton's (1642/43–1727) three laws of motion for reversible dynamical systems:

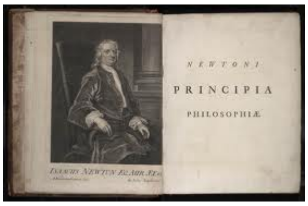

Fig. 2: *Cover of Newton's "Philosophiae Naturalis Principia Mathematica"*

1. *Law of inertia*: The force-free ball moves straight and steadily.
2. *Law of action*: If a force f acts on the ball of mass m, then its acceleration is $a = f/m$.
3. *Law of reaction*: The mutual forces of action and reaction between two bodies are equal, opposite, and collinear.

With his three laws and the introduction of gravitation as a force acting on every mechanical system, Newton modeled the planetary system via the equations of motion in the form

$$M\ddot{x} = F(x),$$

which also describe the motion of our ball. Using his model, Newton obtained many new results and confirmed prior results of Kopernikus (1473–1543), Galilei (1564–1642), and Kepler (1571–1630).

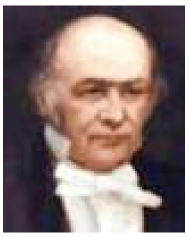

Fig. 3: *Sir William Rowan Hamilton (4.8.1805–2.9.1865)*

Hamilton (1805–1865) realized that the energy, a concept introduced by Leibniz (1646–1716), can be used to rewrite the equation of motion as an energy-driven system. The state $q = (x, p)$ is given in terms of the position x and the momentum $p = M\dot{x}$. The energy is then given in terms of the function $\mathcal{H}(x, p)$, nowadays called Hamilton function:

$$\dot{x} = \partial_p \mathcal{H}(x,p) \text{ and } \dot{p} = -\partial_x \mathcal{H}(x,p) \qquad \text{or} \quad \dot{q} = J\mathrm{D}\mathcal{H}(q) \text{ with } J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \tag{1}$$

A direct consequence of the antisymmetry of J is the conservation of energy along solutions, i. e., $\frac{\mathrm{d}\mathcal{H}(q(t))}{\mathrm{d}t} = \mathrm{D}\mathcal{H}(q(t)) \cdot \dot{q}(t) = \mathrm{D}\mathcal{H}(q(t)) \cdot J\mathrm{D}\mathcal{H}(q(t)) = 0$. This kind of dynamics is often called *re-*

versible, since running the time backwards does not change the system behavior. In particular, the relations (1) reflect that a Hamiltonian system, describing reversible dynamics, is fully governed by the energy that acts as the driving potential of the system.

For our ball, the energy is composed of the kinetic and the potential energy $\mathcal{H}(x,p) = p^2/(2m) - g \cdot x$. Hence, from (1) we obtain $\dot{x} = p/m$ and $\dot{p} = g$, which exacty yields Newton's second law. Furthermore, for $g = 0$ we find that the ball moves steadily as dictated by Newton's first law.

Fig. 4: *The ball as an elastodynamic system*

Now we start bouncing the ball. When hitting the ground, it gets deformed, and when lifting off, it regains its original round shape. Our ball is now an elasto-dynamic system that can be described under consideration of Cauchy's (1789–1857) stress theorem. Instead of the space coordinate x, we introduce the deformation $\varphi : \Omega \to \mathbb{R}^d$. When the ball hits the ground, its impact causes elastic deformations of the ground as well as mechanical stresses inside the ball, which are released again when it lifts off. This deformation leads to additional stored elastic energies $V_{\text{ground}}(\varphi)$ and $W_{\text{def}}(\nabla\varphi)$ such that the total Hamilton function is obtained after integrating over the whole ball Ω, namely $\mathcal{H}_{\text{eldyn}}(\varphi, p) = \int_\Omega H_{\text{eldyn}}(\varphi, \nabla\varphi, p)\mathrm{d}y$ with $H_{\text{eldyn}}(y, \varphi, \boldsymbol{F}, p) = p^2/(2\varrho) + W_{\text{def}}(\boldsymbol{F}) + V_{\text{ground}}(\varphi) - g \cdot \varphi$. Since here also $\boldsymbol{F} = \nabla\varphi$ occurs, the second relation in (1) reads $\dot{p} = -\partial_\varphi \mathcal{H}_{\text{eldyn}}(\varphi, \boldsymbol{F}, p) + \operatorname{div}\left(\partial_{\boldsymbol{F}} \mathcal{H}_{\text{eldyn}}(\varphi, \boldsymbol{F}, p)\right)$ by using the variational derivative.

After throwing and bouncing the ball, we play with it in the bath tub. Watching it float on the hot water surface, we wonder about the temperature changes inside and about possible chemical reactions activated by these temperature changes. In 1852, already William Thomson (1824–1907, later Lord Kelvin) observed that the absorption of radiant heat in a chemical reaction causes dissipation of mechanical energy, and perfect restoration is impossible. Hence, reversing the time does not recover the original system, which explains why these systems are called *irreversible*.

Fig. 5: *Lars Onsager (27.11.1903–5.10.1976)*

Inspired by the works of Thomson, Lars Onsager (Figure 5) stated in [1]: "When two or more irreversible transport processes ... take place simultaneously in a thermodynamic system the processes may interfere with each other. ... In such cases one may naturally suspect reciprocal relations by analogy to the reciprocal relations which connect forces and disclacements in the equilibrium theory of mechanics and thermodynamics." In his work, for which he was awarded with the Nobel Prize in Chemistry in 1968, he derived a general class of reciprocal (=symmetry) relations in irreversible processes from the assumption of microscopic reversibility. Moreover, he stated that for irreversible, non-isothermal processes, it is the entropy that acts as a driving functional. Putting these facts together, the rate of change of a state q obeys the equation

$$\dot{q} = K\mathrm{D}\mathcal{S}(q), \qquad \text{where } K \text{ is symmetric and positive semidefinite.} \tag{2}$$

It was only recently realized by Felix Otto (Max Planck Institute for Mathematics in the Sciences, Leipzig; cf. [4]) that the heat equation can be formulated as a gradient system driven by the physical entropy, namely in terms of the so-called *Wasserstein approach*. This gradient structure was generalized to describe the reaction-diffusion processes in [3]. In particular, it is advantageous to use the corresponding dual formulation (2) involving the entropy functional $\mathcal{S}$ and the *Onsager operator* $K(q)$, which often is a sum of several irreversible processes such as $K(q) = K_{\text{diff}}(q) + K_{\text{react}}(q)$ for reaction-diffusion systems, where K_{diff} contains differential operators like $-\operatorname{div}(\mathbb{M}(q)\nabla\square)$ where "$\square$" stands for the argument. To highlight the duality between reversible and irreversible effects, we call the irreversible system (2) an *Onsager system*.

Fig. 6: *The ball as a GENERIC system*

Finally, we push our ball under the surface of hot water and squeeze it. To understand the new coupled effects we need to couple the Onsager system for the temperature changes and chemical reactions with the Hamiltonian system for the elastic oscillations of the ball. Systematic treatments of the interplay between reversible and irreversible dynamics were only studied since the 1980's. From these results, Öttinger and Grmela [2] developed the concept of GENERIC that combines these two types of dynamics in a particular way.

To keep this presentation short, we will treat thermodynamically closed systems only, i. e., systems that exchange neither matter nor heat with their surroundings. Hence, there are no boundary fluxes and, therefore, all boundary integrals are 0.

The mathematical building blocks of GENERIC: Hamiltonian and Onsager systems

The fundamental ingredients of GENERIC are Hamiltonian systems for reversible dynamics and Onsager systems for irreversible dynamics. Both are formulated on a state space $\mathcal{Q}$ via a driving potential $\Phi : \mathcal{Q} \to \mathbb{R}$ and a geometric structure. For simplicity, we assume that $\mathcal{Q}$ is a Banach space with dual pairing $\langle \cdot, \cdot \rangle$. The driving force is given by the functional derivative $\mathrm{D}\Phi(q) \in \mathcal{Q}^*$.

Hamiltonian systems $(\mathcal{Q}, \mathcal{E}, J)$. In the spirit of Hamiltonian mechanics, a general Hamiltonian system accounts for reversible dynamics only. The equations of motion are given by $\dot{q} = J\mathrm{D}\mathcal{E}(q)$. The driving potential of reversible dynamics is the energy of the system $\mathcal{E} : \mathcal{Q} \to \mathbb{R}$, which may comprise kinetic, mechanical, and thermal energy. The defining property for a Hamiltonian system is that J is a *Poisson structure*, which means that

$$J \text{ is antisymmetric, i. e., } J = -J^*, \text{ and } J \text{ satisfies Jacobi's identity.} \tag{3}$$

The latter property relates to the Poisson bracket $\{\cdot, \cdot\}$ defined via $\{\Phi_1, \Phi_2\} := \langle \mathrm{D}\Phi_1, J\mathrm{D}\Phi_2 \rangle$ for all $\Phi_j : \mathcal{Q} \to \mathbb{R}$. Jacobi's identity means $\{\Phi_1, \{\Phi_2, \Phi_3\}\} + \{\Phi_3, \{\Phi_1, \Phi_2\}\} + \{\Phi_2, \{\Phi_3, \Phi_1\}\} = 0$ for all $\Phi_1, \Phi_2, \Phi_3 : \mathcal{Q} \to \mathbb{R}$. The antisymmetry of J ensures conservation of energy.


Fig. 7: *Deformation of the ball*

As an example we consider the elastodynamics of our ball. The states $q = (\varphi, p)$ are given by the deformation $\varphi : \Omega \to \mathbb{R}^3$ and the momentum $p = \varrho\dot{\varphi}$ with ϱ as the mass density and $\Omega \subset \mathbb{R}^3$ as the reference domain. The energy of the system is composed of the kinetic energy, the stored elastic energy, and the energy due to the external forces, i. e., $\mathcal{E}(q) := \int_\Omega H_{\mathrm{eldyn}}(\varphi, \nabla\varphi, p)\,\mathrm{d}y$, where H_{eldyn} is as above. For J as in (1), the equations of motion $\dot{q} = J\mathrm{D}\mathcal{E}(q)$ read $\dot{\varphi} = \delta_p E = p/\varrho$ and $\dot{p} = -\delta_\varphi E = \operatorname{div}\left(\partial_{\boldsymbol{F}} W_{\mathrm{def}}\right) + \partial_\varphi V_{\mathrm{ground}} + g$. The first equation is just the definition of the momentum. It is $\dot{p} = \varrho\ddot{\varphi}$ and, hence, the second equation is the dynamic force balance of continuum mechanics.

Onsager systems $(\mathcal{Q}, \mathcal{S}, K)$. An Onsager system is related to the dynamics of irreversible, dissipative effects. The evolution equations read $\dot{q} = K(q)\mathrm{D}\mathcal{S}(q)$. The driving functional is the total entropy $\mathcal{S}$, and the the geometric structure is the so-called *Onsager operator*:

$$K \text{ is symmetric, } K = K^*, \text{ and positive semidefinite, } \langle \xi, K\xi \rangle \geq 0\,. \tag{4}$$

While the positive semidefiniteness is a manifestation of the second law of thermodynamcis, the symmetry of K is a generalization of Onsager's reciprocal relations. The properties of K are equivalent to assuming the existence of a nonnegative dual entropy-production potential $\Psi^* = \Psi^*(q,\xi) = \frac{1}{2}\langle \xi, K(q)\xi\rangle$, which is quadratic in the thermodynamic driving force $\xi \in \mathcal{Q}^*$. More generally, $\Psi^*(q,\cdot)$ can be nonquadratic, but nonnegative, convex, and satisfying $\Psi^*(q,0) = 0$. Then, the evolution reads $\dot{q} = \mathrm{D}_\xi \Psi^*(q, \mathrm{D}\mathcal{S}(q))$. This is, e. g., the case for generalized standard materials with a rate-independent evolution of the internal variable, where $\Psi^*(q,\cdot)$ is positively 1-homogeneous. For further details we refer to [5].

Following [2], we consider a reaction-diffusion system with the reaction $N_2 + 3\,H_2 \rightleftharpoons 2\,NH_3$. Denoting the densities of N_2, H_2, and NH_3 by u_1, u_2, and u_3 (relative to the equilibrium densities), and by m_j the corresponding mobilities, we obtain the system

$$\begin{pmatrix} \dot{u}_1 \\ \dot{u}_2 \\ \dot{u}_3 \end{pmatrix} = \begin{pmatrix} m_1 \Delta u_1 \\ m_2 \Delta u_2 \\ m_3 \Delta u_3 \end{pmatrix} + k(u)\,(u_1 u_2^3 - u_3^2) \begin{pmatrix} -1 \\ -3 \\ 2 \end{pmatrix}.$$

Fig. 8: Reaction-diffusion system

To highlight the general usability of Onsager systems, we note that this reaction-diffusion system is a true Onsager system for the relative entropy $\mathcal{S}$ and the entropy-production potential Ψ^*

$$\mathcal{S}(u) = -k_\mathrm{B} \int_\Omega u_1 \log u_1 - u_1 + u_2 \log u_2 - u_2 + u_3 \log u_3 - u_3 \,\mathrm{d}y,$$

$$\Psi^*(u,\mu) = \frac{1}{k_\mathrm{B}} \int_\Omega \sum_{j=1}^{3} \frac{m_j u_j}{2} |\nabla \mu_j|^2 + k(u)\,\Lambda(u_1 u_2^3, u_3^2)\,(\mu_1 + 3\mu_2 - 2\mu_3)^2 \,\mathrm{d}y,$$

where $\Lambda(a,b) = (a-b)/(\log a - \log b)$. For more general reaction-diffusion systems, also including heat conduction and electric charges, we refer to [3].

GENERIC combines reversible and irreversible dynamics

A GENERIC system is a quintuple $(\mathcal{Q}, \mathcal{E}, \mathcal{S}, J, K)$ where the triple $(\mathcal{Q}, \mathcal{E}, J)$ is a Hamiltonian system and $(\mathcal{Q}, \mathcal{S}, K)$ is an Onsager system. The combined evolution equations have the form

$$\dot{q} = J(q)\mathrm{D}\mathcal{E}(q) + K(q)\mathrm{D}\mathcal{S}(q), \tag{5}$$

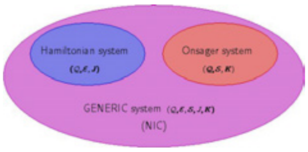

Fig. 9: GENERIC systems

which clearly shows the reversible and the irreversible part of the dynamics. However, there is a crucial and nontrivial coupling condition, which we call

noninteraction condition (NIC): $\quad K\mathrm{D}\mathcal{E} \equiv 0 \quad$ and $\quad J\mathrm{D}\mathcal{S} \equiv 0$. (6)

On the one hand, these conditions ensure energy conservation and entropy production; see [2, 5]. On the other hand, (6) guarantee the validity of the maximum entropy principle, i. e., if q_* maximizes $\mathcal{S}$ subject to the constraint $\mathcal{E}(q) = E_0$, then q_* is a steady state of (5).

Fig. 10: A biomechanical system

Biomechanics as an example. GENERIC systems facilitate the coupling of heat conduction, chemical reactions, diffusion, and elastodynamics, which are important features in growing biomaterials such as bones or wood. For the states $q = (\varphi, p, u, \theta)$, the total energy $\mathcal{E}$ is defined via the density $E(\varphi, \nabla\varphi, p, u, \theta) = |p|^2/(2\varrho) + W(\nabla\varphi, u, \theta) - f \cdot \varphi$, and the total entropy is $\mathcal{S}(q) = \int_\Omega S(\nabla\varphi, u, \theta)\mathrm{d}y$. The Poisson structure is defined by $J = M_{\mathcal{S}} J_0 M_{\mathcal{S}}^*$, where

$$M_{\mathcal{S}} := \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & I & 0 \\ -\frac{\partial_{\boldsymbol{F}} S:\nabla\Box}{\partial_\theta E} & 0 & \frac{-\partial_u S\cdot\Box}{\partial_\theta S} & \frac{1}{\partial_\theta S} \end{pmatrix}, \quad J_0 := \begin{pmatrix} 0 & I & 0 & 0 \\ -I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad M_{\mathcal{S}}^* := \begin{pmatrix} I & 0 & 0 & -\mathrm{div}\big(\frac{\Box}{\partial_\theta S}\partial_{\boldsymbol{F}} S\big) \\ 0 & I & 0 & 0 \\ 0 & 0 & I & \frac{-\Box}{\partial_\theta S}\partial_u S \\ 0 & 0 & 0 & \frac{1}{\partial_\theta S} \end{pmatrix}$$

with $\boldsymbol{F} = \nabla\varphi$. When applying the matrix operators to a vector, □ has to be replaced by the corresponding vector component. The Onsager operator is given by $K = N_{\mathcal{E}} K_0 N_{\mathcal{E}}^*$ with

$$N_{\mathcal{E}} = \begin{pmatrix} I & 0 & 0 & 0 \\ 0 & -\mathrm{div} & 0 & 0 \\ 0 & 0 & I & 0 \\ \frac{-\partial_{\boldsymbol{F}} E:\Box}{\partial_\theta E} & \frac{-(\nabla\partial_p E):\Box}{\partial_\theta E} & \frac{-\partial_u E\cdot\Box}{\partial_\theta E} & \frac{1}{\partial_\theta E} \end{pmatrix}, \quad N_{\mathcal{E}}^* = \begin{pmatrix} I & 0 & 0 & \mathrm{div}\big(\frac{\Box}{\partial_\theta E}\partial_{\boldsymbol{F}} E\big) \\ 0 & \nabla & 0 & \frac{-\Box}{\partial_\theta E}\dot{\boldsymbol{F}} \\ 0 & 0 & I & \frac{-\Box}{\partial_\theta E}\partial_u E \\ 0 & 0 & 0 & \frac{1}{\partial_\theta E} \end{pmatrix},$$

$$K_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & K_{\mathrm{visc}} & 0 & 0 \\ 0 & 0 & K_{\mathrm{react}} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -\mathrm{div}(\mathbb{M}_{uu} : \nabla\Box) & -\mathrm{div}(\mathbb{M}_{u\theta}\nabla\Box) \\ 0 & 0 & -\mathrm{div}(\mathbb{M}_{u\theta}^* : \nabla\Box) & -\mathrm{div}(\mathbb{M}_{\theta\theta}\nabla\Box) \end{pmatrix},$$

where K_0 displays the viscoelasticity through K_{visc}, the reactions through K_{react}, and the diffusion through $\mathbb{M}$. The evolution equation $\dot{q} = M_{\mathcal{S}} J_0 M_{\mathcal{S}}^* \mathrm{D}\mathcal{E}(q) + N_{\mathcal{E}} K_0 N_{\mathcal{E}}^* \mathrm{D}\mathcal{S}$ takes the form

$$\begin{aligned} \dot{\varphi} &= \partial_p E = p/\varrho\,, \\ \dot{p} &= \mathrm{div}\,\big(\partial_{\boldsymbol{F}} W - \tfrac{1}{\theta}\partial_{\boldsymbol{F}} S + K_{\mathrm{visc}}\nabla\dot{\varphi}\big) + f\,, \\ \dot{u} &= -\,\mathrm{div}\,\boldsymbol{j}_u + K_{\mathrm{react}}\big(\partial_u S - \tfrac{\partial_\theta S}{\partial_\theta E}\partial_u E\big)\,, \\ \dot{\theta} &= -\tfrac{1}{\partial_\theta E}\,\mathrm{div}\,\boldsymbol{j}_\theta + \tfrac{1}{\partial_\theta E}\partial_u E \cdot \Big(\mathrm{div}\,\boldsymbol{j}_u - K_{\mathrm{react}}\big(\partial_u S - \tfrac{\partial_\theta S}{\partial_\theta E}\partial_u E\big)\Big)\,, \end{aligned}$$

where $\partial_\theta S/\partial_\theta E = 1/\theta$ by the Gibbs relation, $\boldsymbol{j}_u = \mathbb{M}_{uu}\nabla\big(\partial_u S - \frac{\partial_\theta S}{\partial_\theta E}\partial_u E\big) + \mathbb{M}_{u\theta}\nabla\big(\frac{\partial_\theta S}{\partial_\theta E}\big)$, and $\boldsymbol{j}_\theta = \mathbb{M}_{u\theta}^*\nabla\big(\partial_u S - \frac{\partial_\theta S}{\partial_\theta E}\partial_u E\big) + \mathbb{M}_{\theta\theta}\nabla\big(\frac{\partial_\theta S}{\partial_\theta E}\big)$. The noninteraction condition (6) $J\mathrm{D}\mathcal{S} \equiv 0 \equiv K\mathrm{D}\mathcal{E}$ follows from the special form of J and K, since $M_{\mathcal{S}}^*\mathrm{D}\mathcal{S} = (0,0,0,1)^\top$ and $N_{\mathcal{E}}^*\mathrm{D}\mathcal{E} = (0,0,0,1)^\top$, while $J_0(0,0,0,1)^\top \equiv 0$ and $K_0(0,0,0,1)^\top \equiv 0$.

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2.4 Nonlinear Optics in the Filamentation Regime

Carsten Brée

Femtosecond filaments are self-organized structures of free electric charges and intense laser light in a transparent medium [1]. They can extend over longitudinal distances of up to some 100 meters, while keeping a near-constant transverse diameter of only some ten to hundred micrometers. In spite of their steady visual appearance (see Figure 1), they actually consist of optical pulses with durations of only some 10^{-15} seconds that come close to the idea of light bullets, conveying concentrated electromagnetic energy at high intensities over kilometer distances. With an electric field strength in these pulses that is comparable to the atomic field strength, exceeding that within lightnings by about a million times, the fundamental laws of linear optics, which govern our everyday's visual experience, do no longer apply.

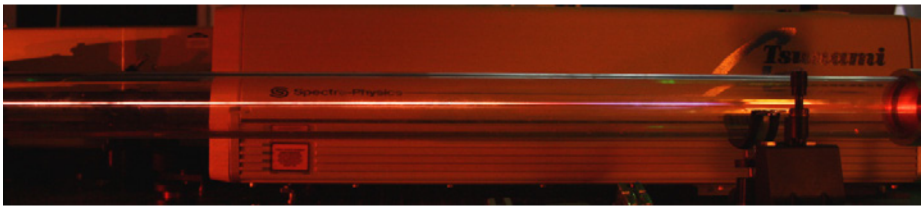

Fig. 1: *A femtosecond filament in an argon-filled gas cell. Experiment conducted at Max Born Institute, Berlin.*

While in linear optics, optical components, like mirrors, gratings, or lenses, are used to influence both spatial beam parameters and temporal pulse shapes, in nonlinear optics the enormous electric field strengths arising within filaments modify the optical properties of the propagation medium and lead to an effective self-interaction of light. This process can result in a self-focusing action, which causes a self-induced narrowing of the spatial beam waist during propagation and is the driving force behind the observed long-range propagation property of filaments. In the time domain, nonlinear effects may lead to temporal self-compression, i. e., to a decrease of the pulse duration during filamentary propagation.

By now, filaments have found widespread applications, including the generation of terahertz radiation, laser-induced breakdown spectroscopy for a highly resolved remote characterization of atomic or molecular emission lines, and the detection of atmospheric trace gases or aerosols by means of LIDAR (Light Detection And Ranging). During the outbreak of the Icelandic volcano Eyjafjallajökull in early 2010, the LIDAR technique was applied for remotely sensing the volcanic ash concentration in the atmosphere.

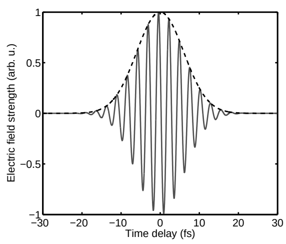

Fig. 2: *Oscillating electric field of an optical pulse (solid line) and envelope (dashed line) versus time*

The research on this topic was performed in the framework of an interdisciplinary project, funded by DFG, that included both theoretical investigations at WIAS and experiments at the Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin. The project aims at a thorough theoretical understanding of the phenomena accompanying femtosecond filamentation. The theory is here of particular importance; due to the extreme field strengths that exceed the damage threshold of any known material, the evolution of optical pulses in the filamentary channel is not accessible to direct measurement. This obvious gap can be bridged by theoretical modeling and numerical simulations that provide a deeper insight into the processes of filamentary dynamics.

The simulations carried out within this project were implemented using a massively parallelized algorithm executed on a compute cluster. Moreover, in certain limiting cases the evolution equation governing femtosecond filaments reduces to a generalized nonlinear Schrödinger equation, allowing even for an exact analytical treatment. Stable nonlinear attractors in such systems offer an explanation for the observed self-healing properties of femtosecond filaments investigated within this project. These tasks are fulfilled in close cooperation with the Max Planck Institute for the Physics of Complex Systems in Dresden and CEA (Commissariat à l'Énergy Atomique) in Paris.

Nonlinear envelope equation

In the filamentary regime at high optical field strengths, the evolution of the electromagnetic field is, in principle, governed by the inhomogeneous Maxwell equations. The derived wave equation for the electric field $\vec{E}$ is a system of hyperbolic partial integro–differential equations of second order in the spatial coordinates x, y, z. The evolution of $\vec{E}$ is coupled to the polarization and the free carrier current, where the former accounts for the bound electron response to the incident optical field, while the latter results from ionization processes. Under certain conditions, Maxwell's equations may be reduced to an equation that is of first order in z, arguing that backscattered radiation is of negligible influence. Providing an initial datum $\vec{E}(x, y, z_0, t)$ for the electric field, i. e., the temporal pulse shape emitted by the laser source, allows a prediction of the evolution of the temporal pulse shape along the longitudinal extension of the filament, usually chosen as the z-direction. As the nonlinear effects within a filament are known to preserve the polarization, we assume a linear polarization of the incident field and switch to a scalar description. Then, an envelope $\mathcal{E}$ is introduced by subtracting the carrier oscillations as suggested by Figure 2. The resulting so-called *nonlinear envelope equation* is widely employed in simulations of femtosecond filaments. It reads

$$\partial_z \mathcal{E} = \frac{i}{2k_0} T^{-1} \Delta_\perp \mathcal{E} + i\mathcal{D}\mathcal{E} + i\frac{\omega_0}{c} n_2 T \int \mathcal{R}(t-t')|\mathcal{E}(t')|^2 dt' \mathcal{E} - i\frac{k_0}{2\rho_c} T^{-1} \rho(\mathcal{E})\mathcal{E}$$
$$-\frac{\sigma}{2}\rho\mathcal{E} - \frac{U_i W(I)(\rho_{nt}-\rho)}{2I}\mathcal{E}, \qquad (1)$$

$$\partial_t \rho = W(I)(\rho_{nt}-\rho) + \frac{\sigma}{U_i}\rho I - \frac{\rho}{\tau_{\mathrm{rec}}} \qquad (2)$$

$$\mathcal{R}(t) = (1-f)\delta(t) + f\theta(t)\frac{1+\omega_R^2\tau_R^2}{\omega_R\tau_R^2} e^{-t/\tau_R} \sin(\omega_R t). \qquad (3)$$

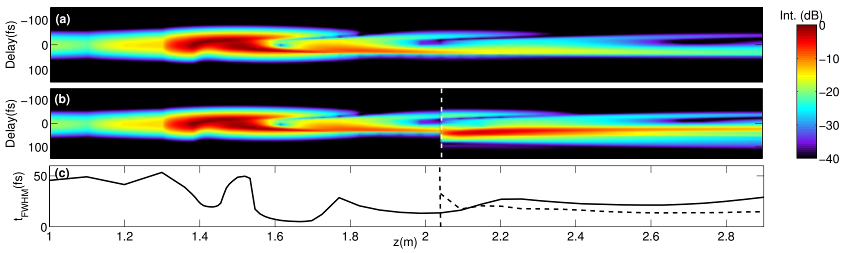

Fig. 3: *(a) Evolution of temporal pulse shape along z in argon (numerics). (b) Same, but with a 0.5-mm-thick silica window located at $z = 2.04$ m. (c) Evolution of pulse duration for windowed (dashed line) and unwindowed (solid line) experimental setup.*

We performed a numerical integration of this system, using a massively parallelized split-step pseudo-spectral method that employs a Crank–Nicolson scheme in the transverse coordinates (x, y), an analytic solution for the dispersive step governed by $\mathcal{D}$, and a Runge–Kutta scheme for the nonlinear propagation along z in the frequency domain.

Nonlinear self-restoration of femtosecond filaments

As a specific feature of nonlinear systems, optical filaments can be shown to exhibit self-healing properties. For example, the transverse spatial profile of a filament can self-restore after a collision with an opaque atmospheric aerosol droplet. Moreover, recent numerical investigations by Skupin et al. [2] suggested that laser pulses that have been self-compressed during filamentary propagation can self-restore their ultrashort temporal characteristics after a sudden nonadiabatic change of both dispersion and nonlinearity that can be realized experimentally by a thin silica exit window inside the gas cell.

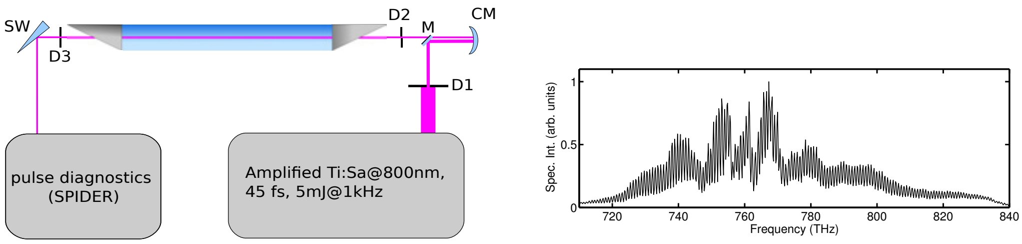

Fig. 4: Left: experimental setup. Right: characteristic fringe pattern obtained from SPIDER measurement.

Using (1)–(3) to simulate the pulse evolution in the gas cell and the subsequent crossing of the silica window, we obtain Figure 3 that details the temporal dynamics of the pulse as it propagates in the gas cell without (a) and with (b) exit window. The vertical dashed line indicates the position of the exit window. Figures 3 (b) and (c) clearly show that the sudden change of nonlinearity and dispersion leads to a significant temporal stretching of the pulse after having crossed the silica sample. However, it is remarkable that, after a further propagation stage of approximately 80 cm, the pulse has nearly restored its original shortness.

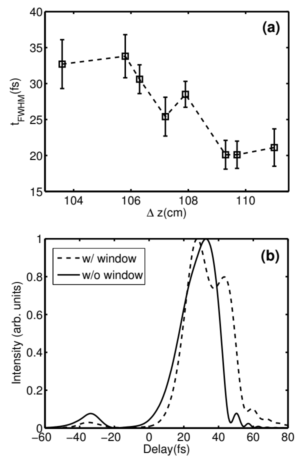

Fig. 5: (a) Measured pulse duration along Δz. (b) Pulse shapes for windowed (dashed line) and unwindowed (solid line) case.

Since in the experiment optical pulses directly within the filament cannot be measured, one has to track the impact of the glass window indirectly. This can be done by longitudinally shifting the gas cell and monitoring the corresponding change of the output pulse emerging from the filament, using the pulse diagnostics located sufficiently remote from the exit window to prevent damage of the apparatus. In order to temporally resolve the optical pulses, an interferometric method (SPIDER) is employed. This method produces a charactistic fringe pattern, cf. Figure 4, whose demodulation to a certain extent allows a reconstruction of the temporal pulse shape. Figure 5 (a) shows the duration of the reconstructed pulses obtained from filamentation in argon for varying gas cell positions Δz. This experimental protocol exhibits the strong impact of the cell position on the pulse shaping dynamics. These measurements provide an experimental evidence of temporal self-restoration and are in good agreement with data from our numerical simulations. The results suggest that the effectivity of temporal self-restoration is strongly sensitive to the longitudinal position of the gas cell, which should be considered as a further parameter in future experiments on filamentary self-compression.

Saturation of the Kerr nonlinear optical response

In linear optics, the refractive index of a medium determines, e. g., the refraction of light at the interface between water and air. The refractive index may depend on the frequency, i. e., the color of the light. This effect is known as dispersion and is responsible for effects leading, e. g., to rainbow formation or the splitting of white light into its spectral components after passage through a prism. However, at extreme field strengths, nonlinear optical effects cause an intensity dependence of the refractive index, in addition to the frequency dependence well known from linear optics. In the so-called *perturbative regime* of nonlinear optics, the intensity-dependent refractive index may be Taylor expanded according to

$$n(I,\omega) = n_0(\omega) + n_2(\omega)I + n_4(\omega)I^2 + n_6(\omega)I^3 + \dots \quad . \tag{4}$$

It is commonly assumed that in this expansion all coefficients $n_4, n_6, \dots$ of order higher than n_2 can be neglected, leading to a linear intensity dependence of the refractive index. Due to this so-called *all-optical Kerr effect*, an intense laser beam modifies the refractive index of the medium to act as a focusing lense. By this effect, the beam will start to self-focus. But, together with the ionization of the medium, a counteracting effect sets in. According to the Drude model, this phenomenon is caused by the defocusing effect of free carriers in the plasma. In fact, the remarkable stability of femtosecond filaments has hitherto been explained by a balance of the focusing Kerr effect and the defocusing plasma effect.

Yet, recent experimental investigations indicated that the all-optical Kerr effect itself may deviate from the linear intensity dependence induced by the n_2 term. Instead, at a certain threshold intensity a saturation starts that eventually leads to a sign change of $\Delta n = n - n_0$, converting the Kerr effect into a defocusing nonlinearity. This unexpected observation initiated an ongoing controversial debate on the nature of the all-optical Kerr effect, since it implies paradigm-changing consequences for our understanding of the physical origins of femtosecond filamentation. In fact, these new experimental findings indicate that defocusing higher-order contributions to the refractive index may balance the self-focusing effect governed by the lowest-order contribution $n_2 I$. This discovery partially contradicts previous beliefs, which mainly assumed plasma defocusing to balance Kerr self-focusing, and leads to the prediction of nearly plasma-free filaments.

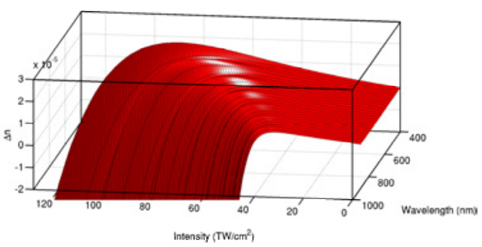

Fig. 6: *Nonlinear refractive index* $\Delta n(I,\omega)$ *versus frequency* ω *and intensity* I

In order to improve the theoretical foundations of the high-order Kerr effect, we extended a method originally developed to calculate the lowest-order term $n_2(\omega)$ and its dispersion in semiconductors. This method relies on the principle of causality that is one of the most fundamental axioms of physics. In optics, this principle requires that the optical response emitted by oscillating atomic dipoles must not depend on future parts of the optical signal. In the frequency domain, the axiom of causality results in the Kramers–Kronig relations between the absorption coefficent $\alpha(\omega)$ and the refractive index $n(\omega)$. While in linear optics it is assumed that each absorbed photon causes precisely one atomic or molecular transition, the intense optical fields relevant in nonlinear optics strongly increase the probability of multiphoton absorption processes. Nevertheless, Kramers–Kronig relations also apply to these nonlinear optical transitions, and our model of the higher-order Kerr effect exploits the fact that the coefficient β_K for K-photon absorption is linked to the coefficients n_{2k} for nonlinear refraction via [5]

$$n_{2k}(\omega) = \frac{c}{\pi}(k+1)\mathcal{P}\int_0^\infty \frac{\beta_{k+1}\left(\frac{\Omega+k\omega}{k+1}\right)}{\Omega^2-\omega^2}d\Omega. \tag{5}$$

Here, as the dominant contribution to multiphoton absorption, we only take into account processes that liberate an electron from the atomic shell, i. e., processes that ionize the medium. While no reliable experimental data on the magnitude of the higher-order coefficients is available, for the lowest-order coefficient n_2, our model yields excellent agreement with reference data. In order to qualitatively compare our results to experimental work [4] and to the saturation and inversion of the Kerr effect observed therein, we calculated n_2 to n_{100} for the noble gases He, Ne, Ar, Kr, and Xe and evaluated the power series (4) for various frequencies ω of the incident field. The results are represented by the surface plot in Figure 6. In fact, for a certain threshold intensity we observe a drastic roll-off of the nonlinear refractive index, leading eventually to a sign change converting the Kerr effect into a defocusing nonlinearity. Further on, the saturation intensity increases for shorter wavelengths. In this way, we provided an efficient method to estimate arbitrary order contributions to nonlinear refraction, which was successfully used to provide theoretical foundations for the experimental finding of [4]. In fact, we predicted comparable threshold intensities for the transition from a focusing to a defocusing Kerr effect as experimentally observed for argon at 800 nm by Loriot *et al.* [4].

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2.5 Compatible Discretizations for Coupled Flow Problems

Alexander Linke and Jürgen Fuhrmann

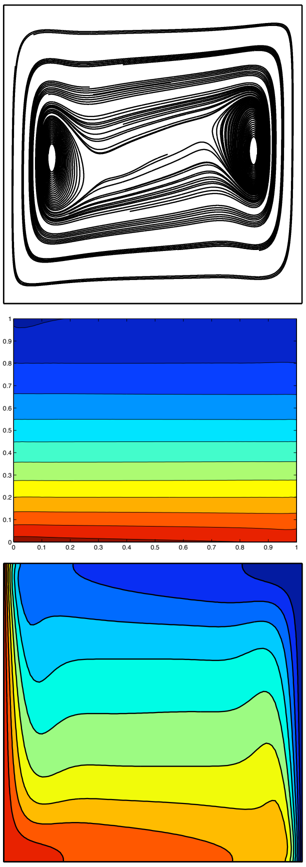


***Fig. 1:** Thermal convection of silicone oil at* $\mathrm{Ra} = 10^6$ *[2]. Top: velocity streamlines, center: pressure, bottom: temperature distribution*

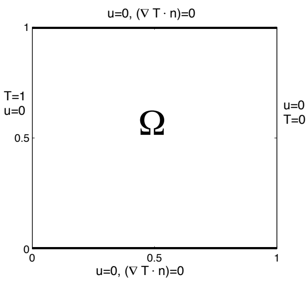


***Fig. 2:** Thermal convection of silicone oil: geometry and boundary conditions for* $\mathbf{u}, T$

The efficient and accurate simulation of coupled flow problems remains a demanding task that is not yet satisfactorily solved in many application fields due to their underlying *multiphysics character*. As a result, on the discrete level the fulfillment of the qualitative structural properties of one subprocess may be influenced by the way how another subprocess is discretized. Available converging coupled methods guarantee that, for fine grid resolutions, all necessary properties are approximated with sufficient accuracy. On coarser and sometimes more realistic levels of resolution, the conformance of the numerical method to certain structural properties of the physical model can result in additional robustness and stability. Such *compatible discretizations* "inherit or mimic fundamental properties of the PDE such as topology, conservation, symmetries, and positivity structures and maximum principles" [1].

Based on finite element or on finite volume methods, compatible discretizations for fluid flow coupled with the transport of a physical quantity (heat, solute) will be presented. It will be discussed which mathematical properties are important for the simulation and how they influence a rigorous numerical analysis of the solution algorithms. Furthermore, it will be demonstrated that a naïve choice of the numerical simulation method for this problem may deliver disappointing results.

Compatible finite element discretizations for the thermal convection of silicone oil in a differentially heated cavity. Here, fluid motion is driven by density differences in the fluid occurring due to temperature gradients, resulting in buoyancy. Therefore, the numerical approximation of the flow has to work accurately in a physical regime that only rarely occurs in pressure-driven flows. The numerical simulation of the temperature distribution has to tolerate that a numerically approximated fluid does not necessarily have all the nice mathematical properties of a "real" fluid.

For small density variations, fluid motion is described by the incompressible Navier–Stokes equations with Boussinesq approximation. Silicone oil is very viscous, therefore the steady incompressible Stokes equations suffice. Buoyancy is modeled by a temperature-dependent forcing in the momentum balance. The temperature evolution is modeled by a conduction-convection equation. The fluid is assumed to be enclosed in a two-dimensional quadratic cavity heated from one side and cooled from the other, with gravity acting in the downward y-direction; see Figure 2. The coupled dimensionless flow problem for the velocity $\mathbf{u}$, the pressure p, and the temperature T reads:

$$-\Delta \mathbf{u} + \nabla p = \mathrm{Ra}\begin{pmatrix} 0 \\ T \end{pmatrix}, \qquad \nabla \cdot \mathbf{u} = 0, \tag{1}$$

$$-\Delta T + \mathbf{u} \cdot \nabla T = 0. \tag{2}$$

Here, Ra is the *Rayleigh number*. Small Rayleigh numbers indicate that the heat transfer is mainly conductive, while large Rayleigh numbers indicate a predominantly convective heat transfer.

Using three different mixed finite element methods, the approximation on the rather coarse mesh shown in Figure 3 is studied. The mixed finite elements studied are the following: the $P_2 - P_1$

mixed finite element using piecewise linear pressure functions that are continuous at the element boundaries (Taylor–Hood element); the P_2–P_0 mixed finite element based on piecewise constant pressures, which thus are discontinuous at the element boundaries; and the P_2–P_{-1} mixed finite element based on piecewise linear pressure functions that, however, will be allowed to be discontinuous at the element boundaries (Scott–Vogelius element). These elements have the same velocity space of piecewise quadratic vector functions that are continuous across element boundaries. They differ only in the pressure space.

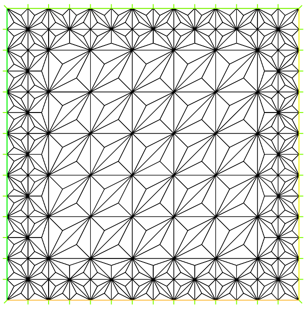
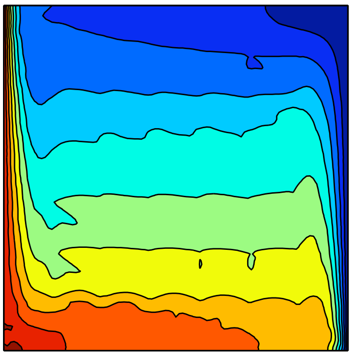
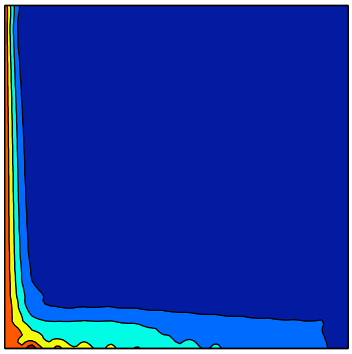


Fig. 3: *Mesh for numerical experiments; see [2]*

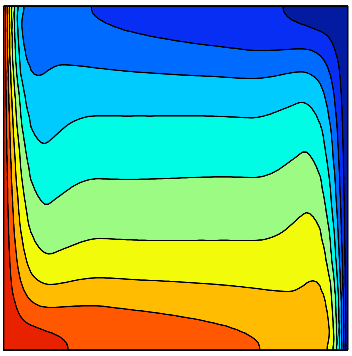
From Figure 4, one obtains that the quality of the simulation results is quite different. The Scott–Vogelius element gives the best result: It is nearly indistinguishable from the fine-grid reference solution. On the same mesh, the Taylor–Hood element delivers significantly less accurate results, and the results from the $P_2 - P_0$ element are far away from the reference solution.



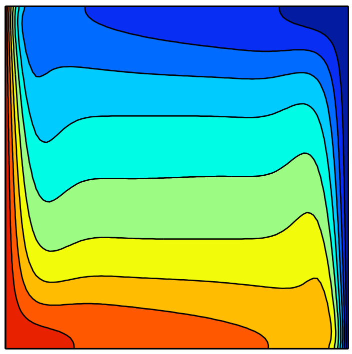
(a) Taylor–Hood $P_2 - P_1$



(b) $P_2 - P_0$ (local mass conservation)



(c) Scott–Vogelius $P_2 - P_1^{\mathrm{disc}}$ (exact mass conservation)



(d) Fine-grid reference solution

Fig. 4: *Simulated temperature profiles for three different finite element methods and reference solution*

The main difference between the Scott–Vogelius element and many other mixed finite element methods for the incompressible Stokes equations is that it delivers exactly divergence-free discrete solutions, i. e., the equation $\nabla \cdot \mathbf{u} = 0$ in (1) also holds for the discrete approximate velocity field. By convergence, the Taylor–Hood method and the $P_2 - P_0$ method guarantee decreasing divergence with finer meshes. But it is hard to control their divergence error on a given particular (coarse) mesh. In our example, the L^2 norm of the divergence error of the Taylor–Hood approximation is about 322, and the corresponding error of the $P_2 - P_0$ approximation about 1915 [2]. Nevertheless, both the Taylor–Hood and the $P_2 - P_0$ methods perform satisfactorily for many problems.

Looking again at the incompressible Navier–Stokes equations (with homogeneous Dirichlet boundary conditions) and forcing $\mathbf{f}$,

$$\mathbf{u}_t - \Delta \mathbf{u} + \mathrm{Re}\,(\mathbf{u} \cdot \nabla)\,\mathbf{u} + \nabla p = \mathbf{f}, \qquad \nabla \cdot \mathbf{u} = 0, \tag{3}$$

one observes that a change of the forcing $\mathbf{f} \to \mathbf{f} + \nabla \varphi$ results in a change of the solution $(\mathbf{u}, p) \to (\mathbf{u}, p + \varphi)$, i. e., the velocity solution $\mathbf{u}$ is invariant with respect to irrotational changes of the forcing, and only the pressure level is affected. In our opinion, this property should not only be considered as an interesting mathematical fact. It has a deeper physical sense, meaning that a conservative forcing does only affect the internal energy of the system, i. e., the pressure, but not the velocity.

For the Scott–Vogelius element, on a given grid, a change of the forcing $\mathbf{f} \to \mathbf{f}+\nabla\varphi$ does not change the discrete velocity solution. In this sense, it can be regarded as a *compatible discretization*. The other two methods (and nearly all other established simulation methods for the incompressible (Navier–)Stokes equations) do not preserve this property.

Due to this compatibility property, for the Scott–Vogelius element the a-priori error estimates for the velocity become completely independent of the pressure and thus can be significantly improved in comparison to those obtained for the competing non-compatible methods.

There are techniques to improve the poor mass conservation of the Taylor–Hood element and of the $P_2 - P_0$ element, e. g., the grad-div stabilization. However, the standard rule of thumb for the choice of the grad-div stabilization parameter $\gamma \sim 1$ is much too optimistic and should be replaced in coupled flow problems by $\gamma \sim \mathrm{Ra}$ [2]. Due to matrix ill-conditioning, this choice can become a problem in computational practice. Moreover, the choice of γ should depend on the ratio $\frac{\mathbf{w}+\nabla\varphi}{\mathbf{w}}$ if $\mathbf{f} = \mathbf{w} + \nabla\varphi$ is orthogonally decomposed by a *Helmholtz–Hodge decomposition* into a divergence-free part $\mathbf{w}$ and an irrotational part $\nabla\varphi$; see [2].

One has to remark that the good performance of the Scott–Vogelius element comes at the expense of stability constraints that require the use of special, barycentrically refined meshes (see Figure 3) and the expensive polynomial degree 3 in three space dimensions. These constraints put serious restrictions on the usability of the element in the general context.

Compatible finite volume discretizations for conduction-convection equations. When considering the influence of a pressure-driven flow on the spatial distribution of the temperature, the local and global maximum principles are of significant interest. Loosely speaking, this means that in the absence of heat sources in the interior of the simulation domain there are no local maxima of temperature, and that its values are bounded by those imposed at the boundary. These properties are directly connected with the condition $\nabla \cdot \mathbf{u} = 0$ in the Navier–Stokes equations (3).

Based on finite element methods for both problems, converging coupling strategies are available. However, mostly they are unable to preserve maximum principles. Even stabilized finite element methods for the conduction-convection equations with pointwise divergence-free velocity are not able to preserve these properties, in general [4]. On the other hand, at the expense of additional meshing constraints, upwind Voronoi finite volume methods guarantee the desired maximum principle if the discrete analogue of the velocity field is divergence-free in a discrete sense.

For a divergence-free $\mathbf{u}$, the conduction-convection equation is written in conservation form

$$\nabla \cdot (-\nabla T + T\mathbf{u}) = 0. \tag{4}$$

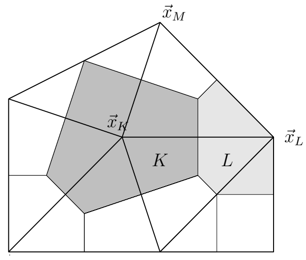


Fig. 5: *Voronoi boxes around discretization points*

Given a partition of Ω into Voronoi cells—see Figure 5 for a two-dimensional example—,one integrates (4) on each cell K, and applies the Gauss theorem to the integral of the flux divergence. Splitting the resulting surface integral into contributions from the facets common with the neighboring control volumes $L \in \mathcal{N}(K)$, applying quadrature rules, and introducing the flux function $g(T_K, T_L, u_{KL})$ to approximate the scaled normal flux between K and L, yields

$$\sum_{L \in \mathcal{N}(K)} \frac{|\partial K \cap \partial L|}{|\mathbf{x}_K - \mathbf{x}_L|} g(T_K, T_L, u_{KL}) = 0. \tag{5}$$

Here, T_K is the average value of T in K, and

$$u_{KL} = \frac{1}{|\partial K \cap \partial L|} \int_{\partial K \cap \partial L} \mathbf{u} \cdot \mathbf{n}_{KL} \, \mathrm{d}s \tag{6}$$

is the average normal flux of $\mathbf{u}$ through $\partial K \cap \partial L$. Any consistent upwind finite difference expression of the flux along $\mathbf{x}_K \mathbf{x}_L$ defines a flux function that leads to a stable and converging scheme. The local and global maximum principles for the discrete solution can be proved provided that the discrete velocities u_{KL} are divergence-free in the discrete sense [3]:

$$\sum_{L \in \mathcal{N}(K)} |\partial K \cup \partial L| u_{KL} \mathbf{n}_{KL} = 0. \tag{7}$$

This condition is fulfilled by projecting a pointwise divergence-free velocity field via (6), allowing for a compatible coupling scheme: First, obtain a pointwise divergence-free discrete velocity field using the Scott–Vogelius mixed finite element. Second, introduce a secondary partition of the domain into Voronoi cells, and obtain discrete velocities by (6). Third, solve the convection-conduction equation using the finite volume scheme (5). This approach leads to a solution of the coupled problem that preserves the maximum principle for temperature. There is no guarantee that the maximum principle is preserved if the discrete velocities are derived, e. g., from the finite element solution of the flow based on the Taylor–Hood element, as was demonstrated in [3]:

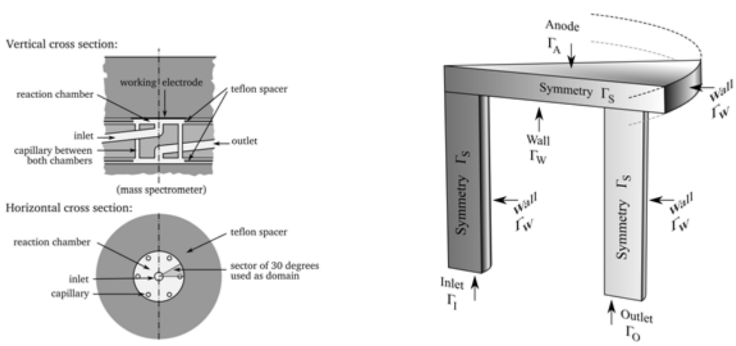


Fig. 6: *Left: Schematic of a thin-layer flow cell. By symmetry, the problem is reduced to the 30 degrees (gray) circular arc shown. Right: computational domain with boundary segments [3].*

Consider a thin-layer flow cell used to perform experimental investigations of catalytic surface reactions; see Figure 6. At the inlet Γ_I, an electrolyte is injected with a hydrogen (H_2) concentration c_I. The part of H_2 reaching the catalyst at Γ_A reacts immediately according to $H_2 \to 2H^+ + 2e^-$. The flow containing the unreacted H_2 leaves the cell at the outlet Γ_O. The transport of the dissolved H_2 is modeled by the same equation (4) as the heat transport.

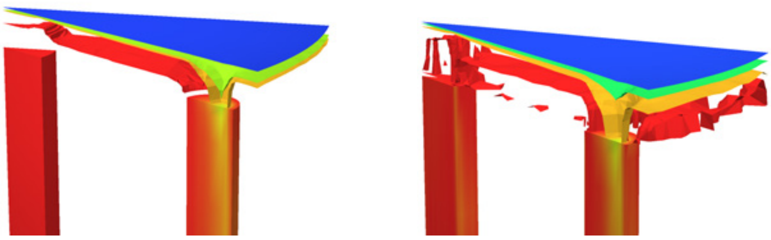


Fig. 7: *Concentration profiles for flow rate* $80\,mm^3/s$ *on a coarse grid: flow calculated using Scott–Vogelius elements (left) and Taylor–Hood elements (right). Isosurfaces are shown in the interior of the working chamber. Color code at surfaces is shown at the inlet and the outlet. Maximum concentration should be 0.62. The red isosurface marks the concentration level 0.6998. [3].*

Figure 7 compares the concentration profiles obtained with the Scott–Vogelius and Taylor–Hood elements, respectively, and highlights the difference concerning the maximum principle.

The control of the solution bounds, both theoretically and numerically, is indispensable whenever considering coupled nonlinear reaction systems where small qualitative errors may accumulate and reaction terms even may become invalid if concentrations leave the domain of definition. At the same time, the preservation of the maximum principle comes at the expense of the convergence rate [5].

Current work includes the investigation of compatible finite volume discretizations of the Navier–Stokes equations [6].

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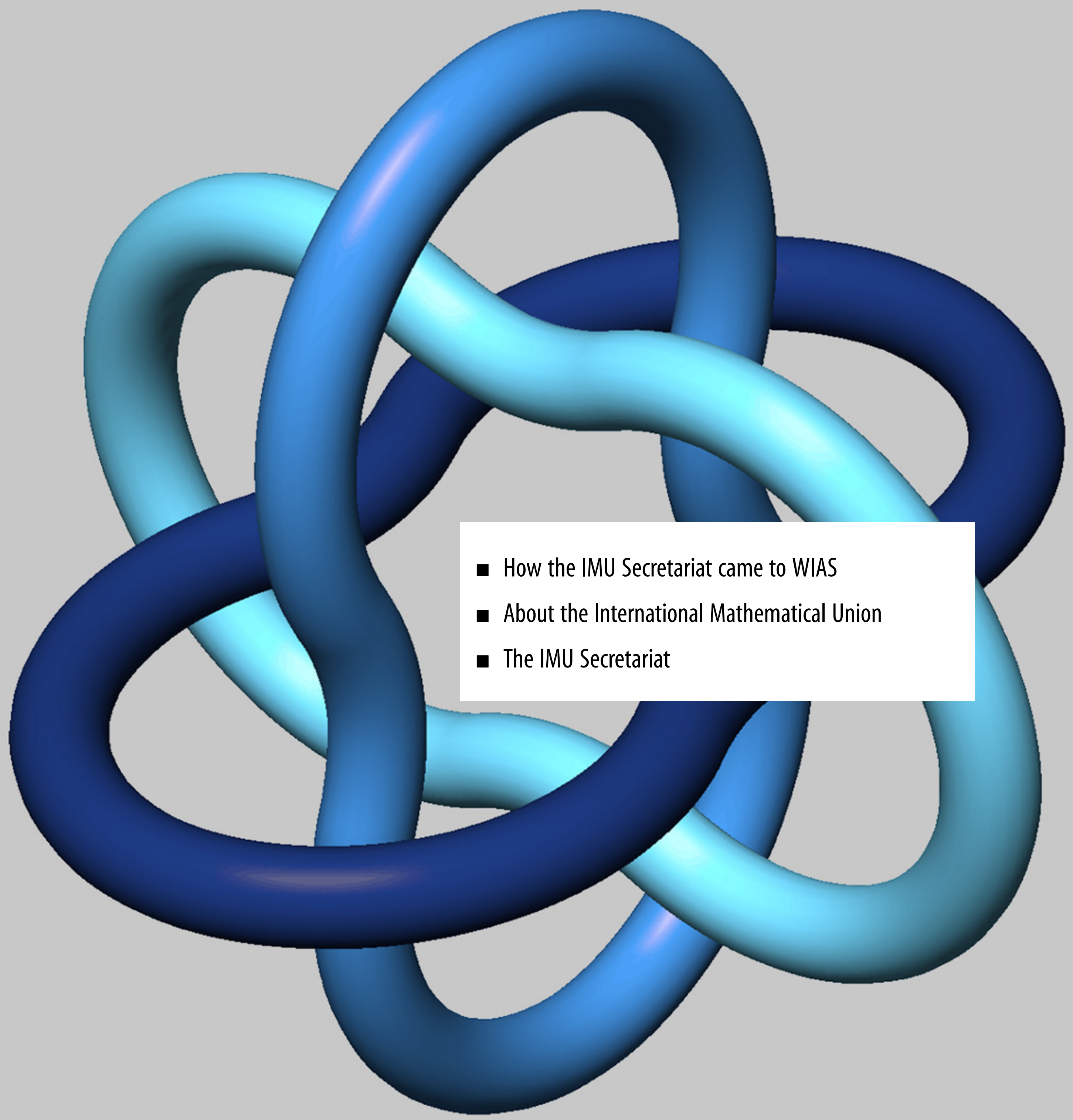
3 IMU@WIAS



- How the IMU Secretariat came to WIAS
- About the International Mathematical Union
- The IMU Secretariat

3.1 How the IMU Secretariat came to WIAS

Alexander Mielke and Sylwia Markwardt

About the selection procedure

The year 2011 is a milestone in the annals of the Weierstrass Institute and of the International Mathematical Union (IMU). This is explained in the following.

In October 2007, the IMU Executive Committee (EC) asked its Adhering Organizations as well as major mathematical societies and institutions to offer suggestions for the location of an office with suitable infrastructure at which the IMU secretarial staff could reside for a longer period of time and at which the costs of running the IMU administrative operations is either low or covered by some long term grant/subsidy or the like. This call was induced by Resolution 11 of the 15th IMU General Assembly, Santiago de Compostela 2006, requesting that the Executive Committee of the IMU "studies the establishment of stable administrative structure and funding mechanisms, including possible fund raising, for the support of the expanding IMU activities, and reports to the 2010 General Assembly with concrete proposals."

Initially, ten institutions had shown an interest in hosting a permanent (stable) office of the IMU. From the remaining six serious proposals by the end of 2008, the so-called *Stable Office Committee* selected three finalists, the Fields Institute, Toronto/Canada, the Instituto Nacional de Matemática Pura e Aplicada (IMPA), Rio de Janeiro/Brazil, and the Weierstrass Institute for Applied Analysis and Stochastics, Berlin/Germany.

Fig. 1: *WIAS presentation to the GA delegates*

At the 16th General Assembly (GA) meeting in Bangalore, India, in 2010, the Fields Institute, IMPA, and WIAS presented their bids to the GA delegates (Figure 1) who had the difficult task to decide whether or not the establishment of a Stable Office for the International Mathematical Union should be endorsed and, if so, to choose among the three excellent proposals. The GA was in favor of a Stable Office, the winner of the vote on the location was WIAS with a fairly clear ballot result.

The decision to permanently locate the office of the IMU at one place was something historic. Since the creation of the contemporary IMU in 1951, the legal domicile of the Union has been moving with the IMU Secretary. This meant that the IMU office has resided in Copenhagen, Rome, Zurich, Paris, Helsinki, Rio de Janeiro, Princeton, and Berlin during these 59 years.

Inauguration of the IMU Secretariat

On January 1, 2011, the International Mathematical Union opened its permanent secretariat at Weierstrass Institute in Berlin. The premises of the secretariat are at Markgrafenstr. 32, 10117 Berlin, Germany (Figure 2, left). The IMU secretariat is supported by a grant of about half a million euros per year provided by the German Federal Ministry of Education and Research (BMBF) and the Berlin Senate. Head of the IMU Secretariat is Professor Alexander Mielke, deputy director of WIAS. Please see page 53 to read about the composition of the secretariat staff (Figure 2, right).

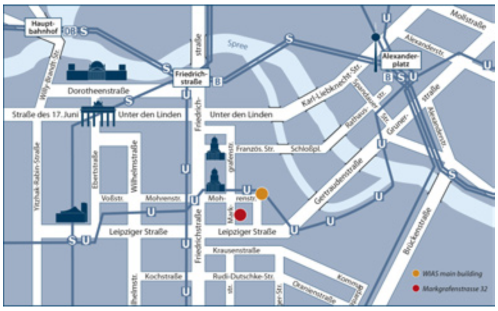


Fig. 2: *Left: IMU Secretariat in Berlin. Right: The team of the permanent IMU Secretariat.*

Under the supervision of the IMU Executive Committee, the secretariat runs IMU's daily business, such as finances and membership handling, and provides support for many IMU operations, including administrative assistance for the International Commission on Mathematical Instruction and the Commission for Developing Countries. The new secretariat also hosts the IMU archive.

The formal opening of the IMU Secretariat was celebrated on February 1, 2011. More than 100 persons from the world over enjoyed the festive event. IMU President Professor Ingrid Daubechies of Duke University (USA), together with Dr. Georg Schütte, State Secretary at the German Federal Ministry of Education and Research, and Dr. Knut Nevermann, State Secretary, Berlin Senate Department for Education, Science and Research, jointly cut a blue ribbon and inaugurated the IMU office (Figure 3).

Fig. 3: *Ribbon Cutting Ceremony*

Highlights of the opening ceremony were speeches delivered by Dr. Georg Schütte, Professor Jürgen Zöllner, Senator for Education, Science and Research of the State of Berlin (speech read by Dr. Knut Nevermann), Professor Ingrid Daubechies, Professor Christian Bär, President of the German Mathematical Society (DMV), and Professor Jürgen Sprekels, Director of the Weierstrass Institute (Figure 4).

The inauguration of the IMU Secretariat at the Weierstrass Institute attracted interest at home and abroad, it was a topic of journals and a news headline of a German TV channel. The IMU Secretary Martin Grötschel and the Head of the IMU Secretariat Alexander Mielke were sought interviewees. The Berlin mathematical community is proud of the fact that the IMU Secretariat is located in Berlin. About 80 professors of mathematics in Berlin who are based in the strong and large mathematical departments of the three major universities Freie Universität (FU), Technische Universität (TU), and Humboldt-Universität (HU), supported the WIAS bid for the Stable IMU Office in Berlin. The IMU gets further support from the Zuse Institute Berlin (ZIB), a mathematical research institute like WIAS, and the Research Center MATHEON of the German Research Foundation and the Excellence Graduate School "Berlin Mathematical School".

Fig. 4: *Impressions from the opening ceremony*

Opening of the IMU archive at the permanent secretariat

It has been mentioned already that the new secretariat also hosts the IMU archive. One room of the secretarial premises was furnished with archive racks and filing cabinets and made ready to store archive material.

The IMU archive has been set up by former IMU Secretary Olli Lehto, Finland. It was hosted and maintained for 17 years at the University of Helsinki. All documents have been moved from Helsinki to Berlin.

Fig. 5: *Workshop "Archiving IMU Material"*

On the occasion of the receipt of the documents and the preliminary set-up of the archive, an opening celebration on a limited scale took place. The *inauguration of the archive* was held on November 10, 2011, in the IMU Secretariat (Figure 6). The archive opening was part of a small workshop entitled "Archiving IMU Material" (Figure 5) where the future organization and format of the archive was discussed. The inauguration was highlighted by the presence of Olli Lehto who gave a very interesting speech, see link[1], about the development of the IMU archive and his personal involvement in the recording of IMU history.

The most important issues of the workshop were how to define an archive database and describing rules, how to organize access to the archive, and how to handle digital material in the archive. Until now, the IMU archive mainly contains paper documents. One priority is to obtain relevant material in electronic form, to find suitable methods of storing and archiving this electronic material.

The archive opening was an excellent occasion to express IMU's gratitude to Olli Lehto and his colleagues at the University of Helsinki for their dedication and permanent service. It is due to them that the IMU archive is in the actual shape.

A "side product" was a video interview with Olli Lehto. This interview is part of a series of interviews taped with presidents and secretaries of the International Mathematical Union. These videos are of great historical value, they will be archived (the suitable format must be specified) and made available as appropriate.

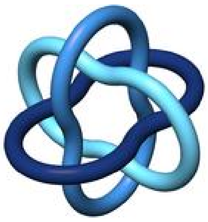
The IMU President Ingrid Daubechies who also attended the archive inauguration and workshop used this opportunity for discussing various ways of implementing the objectives of the Interna-

[1] `http://www.mathunion.org/fileadmin/IMU/Archive/Olli_Lehto_speech.pdf`

tional Mathematical Union. In addition to being present at the archive opening, the IMU President gave a talk at the Berlin Mathematical School within the “Kovalevskaya Colloquium” that emphasizes her activities for women in mathematics. Moreover, this engagement strengthens the interactions between the International Mathematical Union and Berlin mathematics.

Fig. 6: *IMU Archive “Unveiling” Ceremony*

3.2 About the International Mathematical Union



The International Mathematical Union (IMU), a member of the International Council for Science (ICSU), is a non-governmental, non-profit scientific organization.

Objectives:

- Promote international cooperation in mathematics
- Support and assist the International Congress of Mathematicians and other international scientific meetings or conferences
- Encourage and support other international mathematical activities considered likely to contribute to the development of mathematical science in any of its aspects, pure, applied, or educational

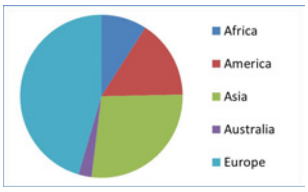


Fig. 1: *Proportional IMU membership distribution*

Structure:

- *Members* are countries who are represented in IMU through Adhering Organizations (AOs). IMU currently has 69 full members, 8 associate members, and 4 affiliate members; see Figure 1.
- IMU's governing body is the *General Assembly (GA)* made up of the AO delegates and representatives and the IMU *Executive Committee* that is elected by the GA and conducts the business of the Union.
- *Commissions and Committees*: International Commission on Mathematical Instruction (ICMI), Commission for Developing Countries (CDC), International Commission on the History of Mathematics (ICHM), and Committee on Electronic Information and Communication (CEIC).
- The permanent *Secretariat*, based in Berlin, runs IMU's day-to-day business, provides support for many IMU operations, and hosts the IMU archive.

  To read more about the personnel associated with the IMU Secretariat, see page 53.

History in a nutshell:

The foundation of IMU was initiated in 1919 and formally completed in 1920 at the International Congress of Mathematicians in Strasbourg. Under difficult political circumstances IMU faded away in the years 1931–1936. IMU came into being again in the years 1950/1952, at the General Assembly in Rome in 1952 the activities of the new Union were inaugurated, the first President and Executive Committee were elected, and IMU was readmitted to ICSU.

The ICM and IMU Prizes. To support and assist the International Congress of Mathematicians (ICM) is an outstanding activity of the IMU. The ICM takes place every four years and unites mathematicians from all its branches and from all over the world. At the ICM Opening Ceremony the scientific prizes of IMU—Figure 2 shows pictures of the obverses of the medals—are awarded:

– *Fields Medal* — for outstanding mathematical achievement for existing work and the promise of future achievement
– *Rolf Nevanlinna Prize* — for outstanding contributions in mathematical aspects of information sciences
– *Carl Friedrich Gauss Prize* — for mathematical research that has had an impact outside mathematics
– *Chern Medal Award* — for accomplishments that warrant the highest level of recognition for outstanding achievements in the field of mathematics

ICMs of recent times were in Beijing (China), 2002, Madrid (Spain), 2006, and Hyderabad (India), 2010. The next ICM will be held in Seoul, Republic of Korea, in 2014. Preregistration is open.

Fig. 2: *Fields, Nevanlinna, Gauss, and Chern medals*

The IMU Executive Committee. The IMU Executive Committee (EC) consists of ten voting members elected for four-year terms: the four officers (president, two vice presidents, and secretary) and six members at large. The retiring president is an ex officio member of the Executive Committee without vote for a period of four years. Figure 3 provides a picture of the current EC.

President:	Ingrid Daubechies (USA)	
Secretary:	Martin Grötschel (Germany)	
Vice Presidents:	Christiane Rousseau (Canada)	Marcelo Viana (Brazil)
Members at Large:	Manuel de León (Spain)	Vasudevan Srinivas (India)
	Yiming Long (China)	John Toland (United Kingdom)
	Cheryl Praeger (Australia)	Wendelin Werner (France)
Ex Officio:	László Lovász (Hungary)	

Fig. 3: *The IMU Executive Committee 2011–2014*

IMU Commissions and Committees and their Objectives.

International Commission on Mathematical Instruction (ICMI)

- Advance the development of mathematical education at all levels, offer a forum to promote reflection, collaboration, exchange and dissemination of ideas on teaching and learning of mathematics
- Facilitate transmission of information on all aspects of theory and practice of contemporary mathematical education from an international perspective
- Link between educational researchers, curriculum designers, educational policy makers, teachers of mathematics, mathematicians, mathematics educators and others

Commission for Developing Countries (CDC)

- Manage, strengthen, and promote the programs of the IMU in developing and economically disadvantaged countries
- Search for funding to support the corresponding activities
- Establish institutional partnerships with scientific organizations with common goals

Fig. 4: *Logos of ICMI, CDC, ICHM, and CEIC*

International Commission on the History of Mathematics (ICHM)

- Inter-union commission joining the International Mathematical Union and the Division of the History of Science (DHS) of the International Union for the History and Philosophy of Science (IUHPS)
- Encourage the study of the history of mathematics
- Promote a high level of historically and mathematically sophisticated scholarship in the field

Committee on Electronic Information and Communication (CEIC)

- Standing committee of the IMU EC with the mandate to advise on matters concerning information and communication
- Review the development of electronic information, communication, publication, and archiving. Publicise relevant developments to the wider community
- Advise about potential opportunities to endorse standards on publication- and communication-related issues, to foster the growth of electronic infrastructure, create tools for this purpose

See the IMU Web site at `http://www.mathunion.org/` for more information.

3.3 The IMU Secretariat

The IMU Secretariat can give a positive summary of its first year of existence at the Weierstrass Institute in Berlin. It has properly fulfilled its responsibilities, that is, assisted the IMU Secretary and the IMU commissions in fulfilling their functions, and accomplished all its other duties. The inauguration of the IMU Secretariat on February 1, 2011, as well as the opening of the IMU Archive on November 10, 2011, were two major events; see page 46.

Below are some details about the team of the IMU Secretariat.

Fig. 1: *The team of the IMU Secretariat*

Head of the IMU Secretariat. Alexander Mielke is Head of the IMU Secretariat and IMU Treasurer. He is a professor at the Humboldt Universität zu Berlin and Deputy Director of WIAS. He was appointed IMU Treasurer 2011–2014 by the IMU Executive Committee. In his function as the head of the secretariat he assumes the personnel responsibility for the staff, as treasurer he is responsible for all financial aspects, including collecting dues, financial reports and drafting the budget of IMU.

Manager of the IMU Secretariat. Sylwia Markwardt's responsibilities include to head and supervise all administrative operations of the secretariat and actively participate in the implementation of the decisions and duties of the IMU Executive Committee and the IMU General Assembly in cooperation with the IMU Secretary, communicate with the IMU member countries, draft written materials, write minutes and reports, supervise the IMU Web site, steer and control the secretariat's business operations and IMU finances, monitor deadlines.

ICMI/CDC Administrator. Lena Koch is primarily responsible for supporting administratively the activities of the Commission for Developing Countries and the International Commission on Mathematical Instruction. She is, in particular, in charge of promoting the work of both commissions, managing their Web presence including public relations and communication, handling grant applications, supporting the Volunteer Lecturing Program as well as other programs in developing countries.

IMU Accountant. Anita Orlowsky is, under the supervision of the IMU Treasurer, in charge of executing the financial decisions of IMU, which includes the budget management of the IMU Secretariat, application for and supervision of third-party funds, handling membership dues, all financial aspects of grants and administering expense reimbursements.

IT Administrator. Holger Kalweit is responsible for running the IT operations of the IMU Secretariat. This includes taking care of running the hardware and software infrastructure, in particular, the IMU server and mailing lists, and planning the extension of IMU's IT services for its members, commissions, and committees.

IMU Archivist. Birgit Seeliger is responsible for the IMU archive and in charge of developing a strategy for preserving and making accessible paper documents, photos, pictures, and IMU artifacts and supporting IMU's decision process concerning the electronic archiving of IMU's steadily increasing amount of digital documents.

The office of DMV (Deutsche Mathematiker-Vereinigung) is next door to the secretariat. The premises of the IMU Secretariat were made available for meetings of the DMV presidium and executive board as well as of the executive committee of the European Mathematical Society (EMS).

Already in its starting year, when long-term planning was not yet possible, the IMU Secretariat hosted several events and had numerous visitors, see below.

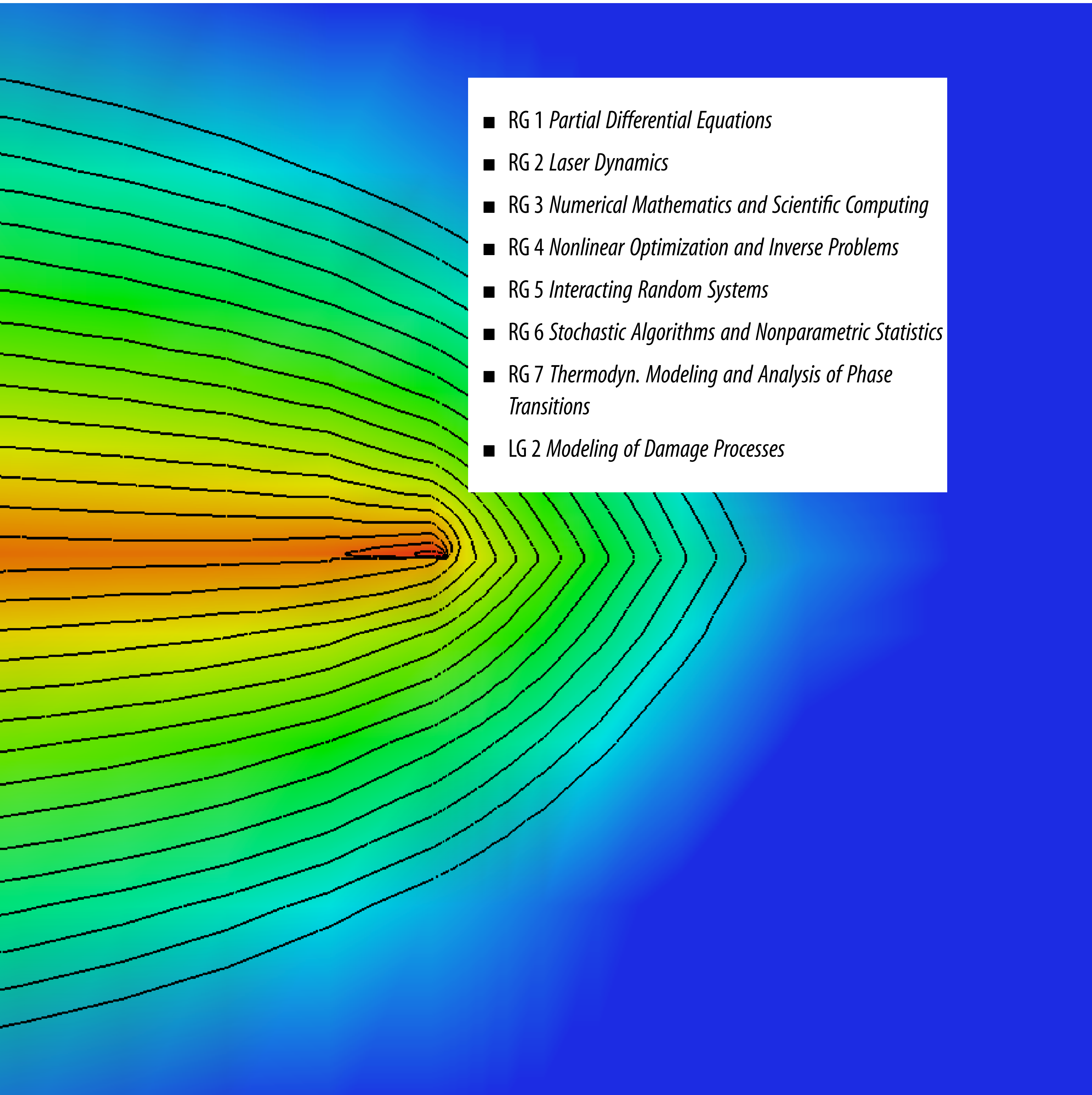
Fig. 2: *Guests at the IMU Secretariat*

Date	Guests	Event
Jan 30–31, 2011 Feb 1, 2011	Michèle Artigue, France; John Ball, UK; Bill Barton, New Zealand; Jaime Carvalho e Silva, Portugal; Herbert Clemens, USA; Ingrid Daubechies, USA; Mama Foupouagnigni, Cameroon; Wanida Hemakul, Thailand; Helge Holden, Norway; Rolf Jeltsch, Switzerland; Srinivasan Kesavan, India; Dongsu Kim, Republic of Korea; László Lovász, Hungary; Daniel Makinde, South Africa; Jarik Nesetril, Czech Republic; Wandera Ogana, Kenya; Hyungju Park, Republic of Korea; José-Antonio de la Peña, Mexico; Hoang Xuan Phu, Vietnam; Ragni Piene, Norway; Chan Roath, Cambodia; Angel Ruiz, Costa Rica; Polly W. Sy, Philippines Dr. Georg Schütte, Federal Ministry of Education and Research, Germany Dr. Knut Nevermann, Berlin Senate Department for Education, Science, and Research, Germany	CDC Meeting IMU Secretariat Inauguration
July 11, 2011	Ingrid Daubechies, USA; Dušanka Perišić, Serbia	Women and Mathematics
Sep 27–Oct 4, 2011	Bill Barton, New Zealand; Jaime Carvalho e Silva, Portugal	ICMI issues
Nov 8/9, 2011	Cedric Villani, France; Ingrid Daubechies, USA	Invited talks
Nov 10, 2011	Guillermo Curbera, Spain; Ingrid Daubechies, USA; Juha Hannikainen, Finland; Olli Lehto, Finland; Tuulikki Makelainen, Finland; Jouni Nikula, Finland	IMU Archive Inauguration, Workshop
Nov 11, 2011	Ingrid Daubechies, USA	Invited talk
Nov 17–23, 2011	Bernard Hodgson, Canada	ICMI Archive
Nov 24, 2011	Olavi Nevanlinna, Finland	BMS, MATHEON
Nov 30, 2011	Philippe Tondeur, USA	Individual visit

Members of the IMU Secretariat participated in several international events, for instance

- IMU EC meeting, Perth, Australia (M. Grötschel, S. Markwardt, A. Mielke)
- IPC meeting for ICME 12, Jeju, Korea; ICMI EC meeting, Beijing, China (L. Koch)
- Former IMU archive at University of Helsinki, Finland (B. Seeliger)
- ERC mathematics representatives meeting, Brussels, Belgium (A. Mielke)
- ICSU General Assembly, Rome, Italy (M. Grötschel, S. Markwardt)

4 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 and Analysis of Phase Transitions*
- LG 2 *Modeling of Damage Processes*

4.1 Research Group 1 "Partial Differential Equations"

The focus of this research group is the analytical understanding of partial differential equations, which 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, also including quantum effects
- Reaction-diffusion systems, also including temperature coupling
- 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 such as Hamiltonian systems and gradient flows or suitable coupled 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.

Qualitative theory for evolutionary systems

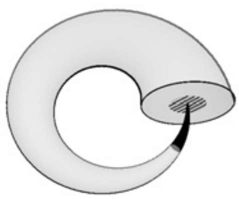


Fig. 1: *A non-Lipschitz domain, where the black apex and the shaded circle carry the Dirichlet condition*

A main field of research is the regularity theory for elliptic and parabolic equations, first in the scalar linear setting and finally for quasilinear systems. In 2011, the group continued a general study on situations where the underlying domain Ω does not have a Lipschitz boundary and the corresponding Dirichlet boundary part may be extremely irregular; see Figure 1. In particular, for such general setting, it was still possible to obtain (i) Hölder continuity, (ii) maximal parabolic regularity, and (iii) useful interpolation results in the Sobolev scale $W^{1,p}(\Omega)$. This result allows the group to provide new existence results for strong solutions for partial differential equations on domains with complicated geometries, in particular, heterostructures, and to treat new applications in optimization or control theory.

In April 2011, the project "Analysis of multiscale systems driven by functionals" started. It is funded by the European Research Council (ERC) as an *Advanced Grant* with a sum of 1.4 million Euros over five years. The project is devoted to evolutionary systems that are defined in terms of energy or entropy functionals and of suitable geometric structures, like Hamiltonian systems, gradient systems, or GENERIC systems, where GENERIC is the acronym for General Equation for Non-Equilibrium Reversible-Irreversible Coupling; see the Scientific Highlights article on page 30. A first multiscale result concerns the derivation of elastoplasticity with rate-independent friction from a purely viscoelastic discrete model with a wiggly energy landscape; see [5]. Another surprising result shows that general Markov processes satisfying the detailed balance condition admit a new gradient structure based on the relative entropy.

Fig. 2: *European Research Council*

Modeling of optoelectronic devices

Since optoelectronic devices are getting smaller and smaller, it becomes desirable to find self-consistent models combining quantum effects and microscopic models on the continuum level.

Quantum mechanical modeling. A first goal is to find good quantum-mechanical models describing light-emitting diodes (LED) or solar cells that are simple enough to be treated in a mathematically rigorous manner. This goal was achieved by coupling leads to a Jaynes–Cummings model describing the interaction of photons and electrons.

The group generalized the abstract Landauer–Büttiker theory under the assumptions that the involved operators are of trace class, which is indeed the case for the proposed model. Thus, the Landauer–Büttiker formula makes it possible to calculate explictly the induced currents and/or the light production rates. Moreover, an appropriate choice of the physical parameters, like the electrochemical potentials and the energy levels of the leads and the light frequency, makes the Jaynes–Cummings system either an LED or a solar cell. The results will be included in the Ph.D. thesis of Lukas Wilhelm.

Photovoltaics. The analytical investigations in the field of thin-film photovoltaics within the MATHEON project D22 "Modeling of electronic properties of interfaces in solar cells" were concentrated on effects of interfaces in semiconductor heterostructures. Models with active interfaces were considered where defects in the interface capture and release charge carriers on their way to the contacts and have an important impact on the electronic properties and the efficiency of the thin-film solar cells. In [1], a gradient structure formulation was found for systems that couple reaction-diffusion effects in bulk and interfaces. Using techniques from [2], coupled bulk-interface models were rigorously derived as limits of bulk models where the thickness of some layers tends to zero. Moreover, existence, boundedness, and uniqueness results for solutions to the model equations with active interfaces were proved in [3].

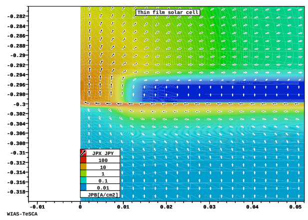


Fig. 3: *Flux density for a structured interface in a heterostructured solar cell simulated by* `WIAS-TeSCA`

Multidimensional simulations for photovoltaic heterostructures with `WIAS-TeSCA` were performed in cooperation with two departments of the Helmholtz Centre Berlin for Materials and Energy, dealing with chalcopyrite and silicon photovoltaics, respectively; see Figure 3. Finally, the research and development project with the company ODERSUN was successfully completed.

Scattering theory for nanowires. The R-matrix formalism is a powerful tool to reduce the computational costs for solving the scattering problem in two- and three-dimensional systems. Indeed, most of the computational time of the R-matrix formalism originates from the Wigner–Eisenbud problem, which is an eigenvalue problem for the electronic Schrödinger operator in an effective mass approximation on a bounded domain with mixed hard- and soft-wall boundary conditions.

The group developed a numerical approach to solve the Wigner–Eisenbud problem based on a two-dimensional Delaunay triangulation of the rotationally symmetric device domain and the finite volume method. Thus, it is possible to describe many complex geometries and to take into account the inhomogeneities and the anisotropy of the material properties, for instance, the effective mass.

Organic semiconducting materials and devices. To enlarge the competence of WIAS in the field of semiconductor applications, jointly with the Research Group *Numerical Mathematics and Scientific Computing* (RG 3), the investigation and numerical treatment of models for organic semiconductor devices was started. Moreover, an intensive collaboration with the Institute for Applied Photophysics of the Technical University of Dresden was initiated.

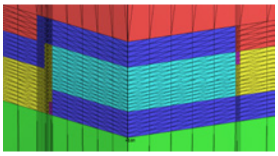


Fig. 4: *Scheme of material composition near heated organic layer (z-coordinate stretched by factor 100)*

One of the novel features of organic semiconducting materials is the increase of the carrier mobility with temperature. This behavior leads to self-amplification of the current and to strong self-heating at locations with large current densities. In order to study heating effects in cross-contacted thin organic layers, comprehensive three-dimensional simulations for the heat flow in crossbar structures were carried out in cooperation with RG 3 using the software `pdelib`; see Figure 5. The difficulty lies in the spatial resolution of the multiple scales inherent to the device structure ranging from 200 nm of the material layer thickness to 200 microns of the contact width; see Figure 4. The results were compared to approximate analytical solutions.

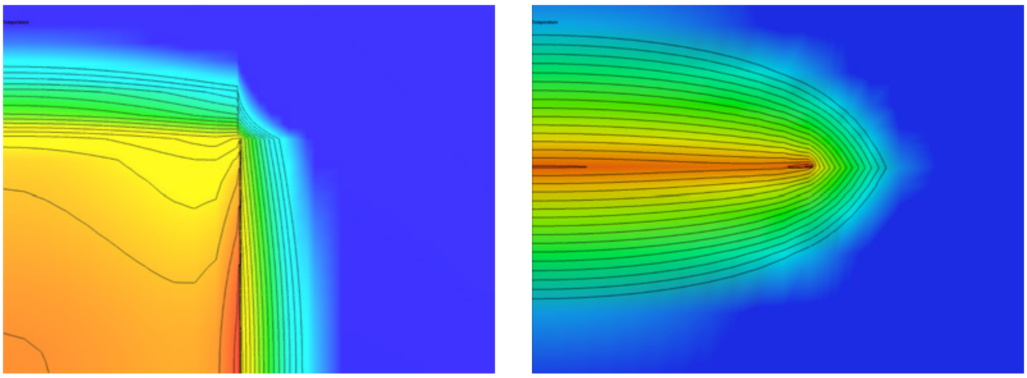


Fig. 5: *Cross sections of the temperature distribution due to volume and edge sources caused by cross currents. Left: horizontal cross section at top contact. Right: vertical cross section.*

Multidimensional modeling and simulation of VCSELs. This grant is sub-project B4 of the DFG Collaborative Research Center (SFB) 787 "Semiconductor Nanophotonics", which has been successful extended to the second funding period 2012–2015. The research on vertical-cavity surface-emitting lasers (VCSELs) is a joint activity of RG 1, RG 2 (*Laser Dynamics*), RG 3, and the Zuse Institute Berlin and is done in cooperation with the Institute of Theoretical Physics at Technische Universität Berlin. A multidimensional multi-species model for lasers with quantum-dot active regions [4] was developed in the first funding period. Results on the electronic properties of prototype VCSEL structures (Figure 6) were obtained with the device simulator `WIAS-Oskar3`; see Figure 7.

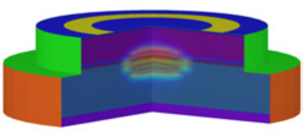


Fig. 6: *3D structure of prototype VCSEL with optical mode intensity*

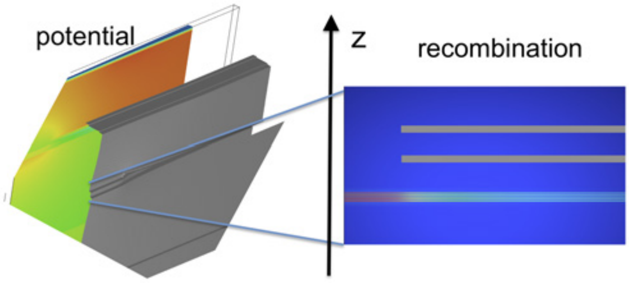


Fig. 7: *Simulation of carrier transport in a prototype VCSEL structure with five active layers with* `WIAS-Oskar3`*. Left: electrostatic potential. Right: rate of radiative recombination.*

Material modeling

The research in this area is devoted to the mathematical modeling and the analysis of solids with elasticity, chemical reactions, and possible additional properties. The focus lies on features that can be described with the aid of internal variables with a viscous or rate-independent evolution. Besides diffusion and reaction of chemical species, this field includes phase transformations, plasticity, and damage and crack propagation, which is investigated in collaboration with the Leibniz Group *Modeling of Damage Processes*.

Shape-memory alloys and elastoplasticity. The MATHEON project C18 "Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys" analyzed several models for shape-memory alloys. The recent research was mainly concerned with the study of non-isothermal models, where the equilibrium of mechanical forces and the transformation rules are coupled with the heat equation in a thermodynamically consistent way, i. e., the latent heat and dissipational heating are properly taken care of.

The sub-project P5 "Regularizations and relaxations of time-continuous problems in plasticity" runs within the DFG Research Unit FOR 797 "Analysis and Computation of Microstructure in Finite Plasticity". One of its main topics is the rate-independent evolution of elastoplastic systems. It is a remarkable result that linearized plasticity, which is well behaved and well posed, can be obtained as the evolutionary Gamma-limit of finite-strain plasticity, although the finite-strain setting exhibits microstructures and non-uniqueness. This result is obtained under the assumption of small yield stresses and very small loadings; see [6].

Alexander von Humboldt Foundation Award Ulisse Stefanelli from the Institute for Applied Mathematics and Information Technologies of the National Research Council (IMATI-CNR Italy), has been honored by the Alexander von Humboldt Foundation with a Friedrich Bessel Research Award to visit WIAS for six months. His stay led to strong collaborations in material modeling, such as the WED approach (Weighted Energy Dissipation), shape-memory alloys, and elastoplasticity; see [6].

Damage models. In the application area of damage, it was possible to generalize the existence results to rate-independent material models with a BV (bounded variation) gradient of the damage variable or even the perimeter as a spatial regularization. This generalization makes it possible to consider material models where the damage variable (or any other internal variable) accounts for two states of the material only: fully intact or maximally damaged. These results will be of importance for the analysis of a model describing rate-independent crack evolution along a prescribed interface in viscoelastic solids with thermal effects.

Pattern formation in reaction-diffusion systems. January 2011 was the start of the Collaborative Research Center (SFB) 910 "Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application", which brings together physisists, chemists, engineers, and mathematicians from various research institutions in Berlin. RG 1 runs the sub-project A5 "Pattern formation in systems with multiple scales". Such multiscale systems do not only arise in composite materials, i. e., in the material modeling of solids, but also in the modeling of biological and chemical processes, e. g., on cell membranes or crystal surfaces. The aim of this project is to investigate the effective influence of microstructure on the formation of macroscopic pattern. This study involves the derivation of effective macroscopic equations for pattern-forming systems by means of multi-scale convergence and homogenization methods. Moreover, it includes the analysis of bifurcations in the effective equations as well as pattern control in both the effective and the original equations.

International conferences

Mathematical Challenges of Quantum Transport in Nano-Optoelectronic Systems. This workshop took place at WIAS on February 4 and 5, 2011, and was partially supported by the DFG. It was organized by Hagen Neidhardt and Paul Racec (both RG 1) in collaboration with Horia Cornean (Aalborg University, Denmark). The 18 talks covered a wide range of mathematically and numerically challenging topics in the field of modeling of semiconductor and optoelectronic quantum devices. In particular, the workshop agenda included quantum dots and nanowires, coupling of light to charge carriers in open quantum systems, and modeling quantum effects in thin-film solar cells.

Autumn School on Mathematical Principles for and Advances in Continuum Mechanics. From November 7 to 12, 2011, an autumn school on "Mathematical Principles for and Advances in Continuum Mechanics" took place at the De Giorgi Center of the Scuola Normale Superiore in Pisa. It was organized by Paolo Maria Mariano (Florence) and Alexander Mielke (RG 1) in the framework of the De Giorgi Activity Group "Theoretical Mechanics". The mini-courses were given by Dick Bedeaux (Trondheim), Paolo Maria Mariano (Florence), Christian Miehe (Stuttgart), Alexander Mielke (RG 1), and Mark A. Peletier (Eindhoven), and each of them presented an in-depth series of lectures. The topics included non-equilibrium thermodynamics of surfaces, variational modeling of materials with length scales, coupling of reversible and irreversible processes in the GENERIC framework, and the stochastic origins of Wasserstein gradient flows. About 30 postdocs and Ph.D. students from Chile, Estonia, France, Germany, Italy, the Netherlands, and Spain enjoyed the casual atmosphere, many stimulating discussions, and the opportunity to exchange their experiences.

Oberwolfach Workshop on Variational Methods for Evolution. This workshop was organized by Alexander Mielke, Felix Otto (Leipzig), Giuseppe Savaré (Pavia), and Ulisse Stefanelli (Pavia) and took place at the Mathematisches Forschungsinstitut Oberwolfach from December 4 to 10, 2011.

Fig. 8: *Organizers: Mielke, Stefanelli, Savaré, Otto*

Fig. 9: *Participants of "Variational Methods for Evolution"*

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[1] A. Glitzky, A. Mielke, *A gradient structure for systems coupling reaction-diffusion effects in bulk and interfaces*, WIAS Preprint no. 1603, 2011, to appear in: ZAMP Z. Angew. Math. Phys., DOI: 10.1007/s00033-012-0207-y.

[2] M. Liero, *Passing from bulk to bulk/surface evolution in the Allen–Cahn equation*, WIAS Preprint no. 1676, 2012, submitted.

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[4] Th. Koprucki, A. Wilms, A. Knorr, U. Bandelow, *Modeling of quantum dot lasers with microscopic treatment of Coulomb effects*, Opt. Quantum Electron., **42** (2011), pp. 777–783.

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[6] A. Mielke, U. Stefanelli, *Linearized plasticity is the evolutionary Gamma-limit of finite plasticity*, to appear in: J. Eur. Math. Soc. (JEMS).

4.2 Research Group 2 "Laser Dynamics"

The focus of this research group is the study of mathematical problems that appear in nonlinear optics and optoelectronics. The research activities include mathematical modeling, theoretical investigation of fundamental physical effects, implementation of numerical methods, efficient modeling and simulation of complex devices, and the development of related mathematical theory, mainly in the field of *dynamical systems*.

The research group contributes to the following application-oriented research topics: *dynamics of semiconductor lasers* and *pulses in nonlinear optical media*.

Highlights in 2011

Fig. 1: *SFB 787 (supported by DFG)*

Successful evaluation of SFB 787. In July 2011, the DFG-funded Collaborative Research Center 787 "Semiconductor Nanophotonics: Materials, Models, Devices" was successfully evaluated. At WIAS, the research in the projects B4 "Multi-dimensional modeling and simulation of VCSEL devices", headed by Uwe Bandelow, Alexander Mielke (Research Group *Partial Differential Equations*), and Frank Schmidt (Zuse Institute Berlin), and B5 "Effective models, simulation, and analysis of the dynamics in quantum-dot devices" headed by Uwe Bandelow and Matthias Wolfrum can now be continued until 12/2015.

Invited SPIE newsroom article on optical transistors. Based on their groundbreaking result published in [1], Shalva Amiranashvili (RG 2) and his collaborators Ayhan Demircan and Günter Steinmeyer (Max Born Institute for Nonlinear Optics and Short-Pulse Spectroscopy (MBI), Berlin) were invited to contribute the highlight article "Optical switching in the event horizon" for the Digital Library Newsroom of the International Society for Optical Engineering (SPIE).

Fig. 2: *The Walton Award is granted by the Science Foundation Ireland (SFI)*

Walton Award for Andrei Vladimirov. The E.T.S. Walton Visitor Awards programme of the Science Foundation Ireland (SFI) is intended to bring high-profile international researchers from academia and industry to Ireland. The award granted to Andrei Vladimirov will deepen the collaboration between WIAS and the Tyndall National Institute and the University College Cork in Ireland. It shows the international visibility of the research group's activities.

Fig. 3: *EU-funded Marie Curie Initial Training Network PROPHET*

Participation in the Marie Curie Initial Training Network PROPHET. PROPHET (Postgraduate Research on Photonics as an Enabling Technology) is an Initial Training Network funded by the EU Framework Programme 7 Marie Curie Actions, which aims to train young researchers in the field of photonics. The research at WIAS will be concerned with theoretical research on dynamics of quantum dot mode-locked lasers and Fourier-domain mode-locked lasers for applications in communication technology as well as in optical coherent tomography.

Dynamics of semiconductor lasers

The research on semiconductor lasers in this research group covers a wide range of devices, including mode-locked lasers, broad area lasers, ring lasers, and VCSELs (vertical cavity surface emitting lasers). Funded projects are carried out in the framework of the DFG Research Center MATHEON, and, as already mentioned above, in the Collaborative Research Center SFB 787 and in the EU-funded Marie Curie Initial Training Network PROPHET. Recently, substantial progress has been achieved in the study of dynamical effects that arise specifically in lasers with quantum-dot active materials [2]; see Figure 4. For these results, the WIAS software `LDSL-tool` has been extended to include the carrier exchange processes between the reservoir and different bound states in the quantum dots. Moreover, using also analytical methods, the effect of injection locking in a mode-locked laser subjected to a single-frequency coherent injection was analyzed.

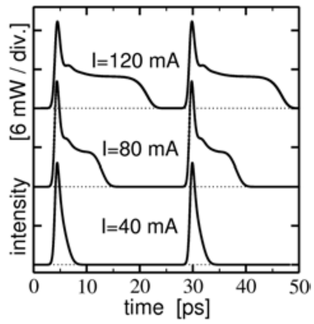

Fig. 4: *Mode-locked quantum-dot laser: pulses with a trailing-edge plateau*

For broad area lasers, a major challenge is the stabilization of the output beam also in the lateral direction. Here, a model was employed that resolves the optical field amplitudes in two spatial dimensions (longitudinal and lateral) and in time, in order to investigate various methods of stabilization suggested by the group's collaboration partners, like off-axis feedback or optical injection.

Pulses in nonlinear optical media

After a series of results on fundamental questions concerning the modeling of short pulses in nonlinear optical media and the mathematical properties of such model equations, Shalva Amiranashvili and his collaboration partners from the Max Born Institute now obtained a result that might also imply far-reaching consequences for future all-optical communication technology. In [1], they reported a scheme for efficient all-optical switching of light pulses, fulfilling all criteria for a practical optical transistor. It is based on a sophisticated setting that enables a strong nonlinear interaction between two pulses in a way that a slightly faster pulse is captured in the nonlinear wake of a stronger pulse traveling ahead, transferring energy from one pulse to the other while conserving the total energy; see Figure 5.

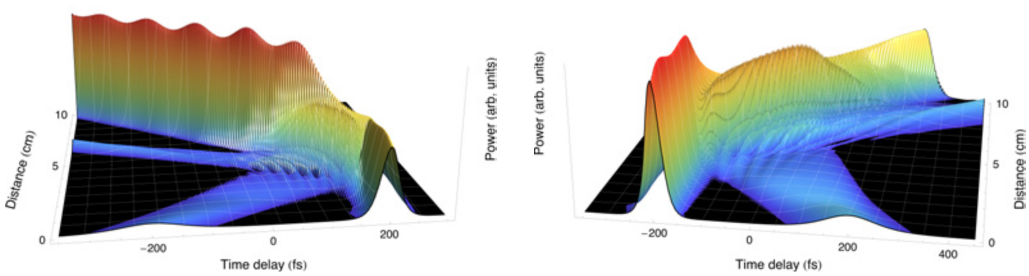

Fig. 5: *On-switching (left) and off-switching (right) of an optical soliton by a weaker dispersive pulse*

A further achievement in this field were the remarkable results in the Ph.D. thesis of Carsten Brée. His dissertation "Self-compression of intense optical pulses and the filamentary regime of nonlinear optics" (awarded *summa cum laude*) is an interdisciplinary work, covering deep theoretical results as well as their experimental realization (at Max Born Institute), and contains results on the saturation of the all-optical Kerr effect [3] with paradigm-changing implications that are currently controversially discussed in physics literature. For more details about his results, see the Scientific Highlights article “Nonlinear Optics in the Filamentation Regime” on page 35.

Dynamical systems

In addition to the application-oriented research mentioned above, the research group contributes also to abstract mathematical theory in the field of dynamical systems. This research contains work on singularly perturbed systems, delay-differential equations, complex and chaotic dynamics in large coupled systems, and the formation and interaction of patterns and pulses. In many cases, it is directly driven by questions arising in the context of the applications. In particular, the feedback and coupling structures of optoelectronic devices inspired the theoretical progress on delay-differential equations in the singular limit of large delay; see [4].

In [5], the stability of clusters of closely packed localized peaks for the Swift–Hohenberg equation in one and two spatial dimensions was studied. The underlying version of the Swift–Hohenberg equation can be considered as a model for interacting solitons in an optical cavity.

Another important event in the previous year was the workshop “Dynamics of Oscillator Populations”, organized together with Serhiy Yanchuk (Humboldt-Universität zu Berlin) and Arkady Pikovsky (Universität Potsdam) in October, where 30 researchers discussed recent developments in this field.

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4.3 Research Group 3 “Numerical Mathematics and Scientific Computing”

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

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 Highlights article on compatible discretizations on page 40.

Modeling of general classical transport processes

Many physical models describing microscopic transport problems, like drift, diffusion, or linear reactions, are well understood. For example, if the motion of a diffusing particle is modeled by means of the Fokker–Planck equation, where the state space is a domain in $\mathbb{R}^n$, it is well known that the probability has a density with respect to the Lebesgue measure. The equation has an equilibrium state, and the solution tends towards this state in time because of a decreasing Lyapunov function (H-theorem).

If the situation is more complicated (heterostructures, various dimensions, a disconnected state space, state space with discrete parts, or degenerate problems), analytical results strongly depend on the mathematical setting.

In [6], an abstract mathematical framework for the modeling of rather arbitrary classical physical transport problems is proposed.

The starting point of the modeling is the definition of the state space $\mathcal{Z}$ and of its topology via a suitably chosen countable set of continuous functions, called *the observables*. In this compact topology, the set of observables is the Banach lattice of continuous functions $\mathcal{C}(\mathcal{Z})$ on $\mathcal{Z}$, i. e, the topological dual of $\mathcal{Z}$, and the statistical state space (probabilities) $\mathcal{S}^*(\mathcal{Z})$ is defined as the weak* closure of the convex hull of the image of the canonical embedding of $\mathcal{Z}$ in its topological bidual space. The change of any statistical state is effected by the adjoint of a Markov operator acting in $\mathcal{C}(\mathcal{Z})$. An evolution equation can be considered in two dual variants: $\dot{g} = \mathbf{A}g$ in a strong sense in $\mathcal{C}(\mathcal{Z})$ or $\dot{p} = \mathbf{A}^* p$ in a weak* sense in $\mathcal{S}^*(\mathcal{Z})$. The proposed framework provides information about the structure of $\mathbf{A}$ so that the evolution equations describe a physically sensible transport process. For example, if $\mathcal{Z}$ is a domain in $\mathbb{R}^m$, the operator $\mathbf{A}$ has to be a pseudo-differential operator of order not greater than 2, i. e., it has on inner points z the structure

$$(\mathbf{A}g)(z) \quad = \quad \sum_{i,j=1}^{m} b_{ij}(z)\frac{\partial^2 g}{\partial z_i \partial z_j} + \sum_{i=1}^{m} a_i(z)\frac{\partial g}{\partial z_i} + \int_{\mathcal{Z}} \big(g(z') - g(z)\big) Q(z, dz'),$$

where $\big(b_{ij}(z)\big)_{i,j=1}^{m}$ is a positive semidefinite matrix and $Q(z,B) \geq 0$ is a nonnegative function defined on all points $z \in \mathcal{Z}$ and Borel sets $B \subset \mathcal{Z}$. The function $Q(z,B)$ can be unbounded for $z \in B$. In this case, the integral operator has to be understood as a principal value integral. If a solution exists, it is unique and global in time.

Regardless of the general setting, important conclusions can be drawn, valid for any physical systems that can be modeled in such a way: There is a large family of Lyapunov functions for any such evolution equation (even if the operator $\mathbf{A}$ depends on time explicitly). This fact is based on some inequalities of Markov operators and their adjoints and illustrates a symmetry break in time that reflects the second law of thermodynamics. Choosing a suitable Lyapunov function from this family, nonlinear thermodynamically consistent macroscopic equations can be derived. If p has a density with respect to a stationary measure μ, i. e., a solution of $\mathbf{A}^*\mu = 0$, this density is a global weak solution in Lebesgue and Marcinkiewicz spaces on μ. Choosing suitable observables, namely a partition of unity of $\mathcal{Z}$, an approximation scheme can be derived that can be understood as a finite physical system with discrete topology.

Numerical methods for transport-dominated scalar equations

Transport-dominated scalar equations are part of coupled systems that are considered in the applications of this research group. For this reason, the development and the study of accurate and efficient numerical methods for this kind of equations is one of the group's main research topics.

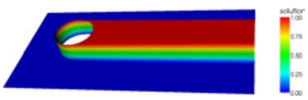

Fig. 1: *Solution of the Hemker example*

In [4], numerical methods for steady-state convection-diffusion equations were assessed that are based on finite element and finite volume ideas. Besides standard methods, like the streamline-upwind Petrov–Galerkin (SUPG) finite element method and an exponentially fitted finite volume scheme, also modern proposals were considered, like a continuous interior penalty (CIP) finite element method, a spurious oscillations at layers diminishing (SOLD) finite element method, a discontinuous Galerkin (DG) finite element method, and a total variation diminishing finite element method (FEMTVD). The assessment was performed on the Hemker example, whose solution is depicted in Figure 1. The solution possesses boundary and interior layers, which is typical for solutions of convection-dominated scalar equations. Quantities of interest that were studied included the size of spurious oscillations, the smearing of layers, and computing times. These quantities are generally of importance in applications. The outcome of the assessment was that each method showed substantial deficiencies in one or the other aspect. None of the methods can be generally recommended for applications. This conclusion emphasizes the need of further research in the development of good discretizations for steady-state convection-dominated problems.

For the SUPG finite element method, the approach for computing an optimal stabilization parameter was pursued, which was described in the Annual Research Report 2010. A key of this approach is the definition of appropriate functionals describing the quality of a computed solution. New functionals were considered that, e. g., include the crosswind derivative of the computed solution;

see Figure 2 for a typical result. The basic ideas and initial numerical results were presented in [1].

Some applications from population balance systems require the solution of time-dependent convection-dominated scalar equations in four-dimensional tensor-product domains. In this situation, the use of finite difference methods is an attractive option. A comparison of essentially non-oscillatory (ENO) and weighted ENO (WENO) finite difference methods with the best finite element method from previous studies was presented in [3]. In these numerical studies, the advantages and drawbacks of the methods became clear, and some recommendations were given concerning the choice of a method for certain situations. Based on the results from [3], the ENO finite difference method combined with a TVD Runge–Kutta scheme became the discretization of choice in the group's simulations of population balance systems.

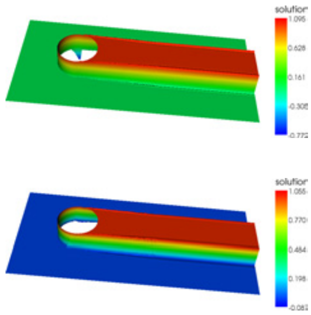

Fig. 2: *Hemker example. Top: SUPG solution with standard parameter containing large spurious oscillations in the layer at the cylinder; bottom: with parameter based on minimizing a functional with crosswind derivative with reduced spurious oscillations in the layer at the cylinder*

Proper orthogonal decomposition for incompressible flows

Proper orthogonal decomposition (POD) is a model reduction technique that aims at finding a lower-order subspace of a given complex set of data that still reflects the most important properties of this set. In connection with numerical methods for the solution of partial differential equations, POD is used to find a lower-dimensional basis able to describe the numerical solution with a certain accuracy.

In the literature, several POD formulations of the Navier–Stokes equations have been described, which, depending on the target application, focus on different treatments of velocity and pressure fields. The implementation of the first POD methods into the code MooNMD has been started in 2011. The aim consists in using these methods for applications with turbulent flows, such as population balance systems.

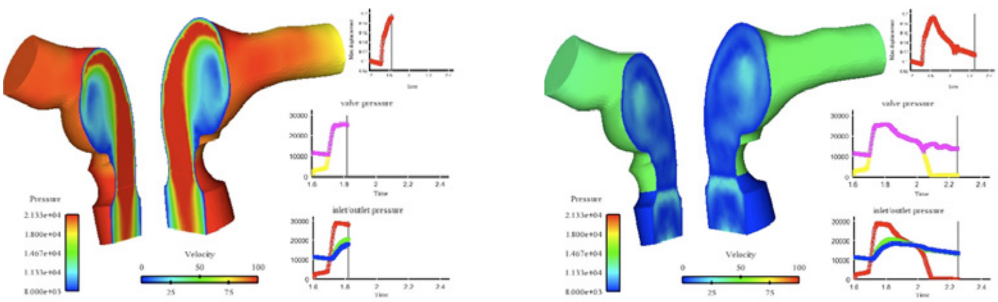

Fig. 3: *Simulation of blood flow in the pulmonary artery using a projection scheme. The pressure (in dyn/cm ^{2}) is shown on the boundary surface, while the velocity scale (in cm/s) refers to the internal cross section. Left: open valve; right: closed valve*

In an on-going research project, in collaboration with the REO team of INRIA Paris-Rocquencourt (head Dr. J.-F. Gerbeau), model-order reduction techniques are investigated for the simulation of the pulmonary artery and the pulmonary valve that combine statistical image analysis and POD; see Figure 3. The current algorithm is based on a projection method for the incompressible Navier–Stokes equations (Chorin–Temam), treating the pulmonary valve as a porous interface [7]. Since the time advancing of the velocity and the pressure field is split into two sub-steps, the projection scheme yields a favorable implementation of a decoupled reduced-order model, where velocity and pressure model reduction can be treated separately. In parallel, the feasibility of Navier–Stokes solvers is addressed where the nonlinear term is treated explicitly, using an additional stabilization term. This approach allows for assembling the finite element matrices only once, thus fully exploiting the potential of model order reduction.

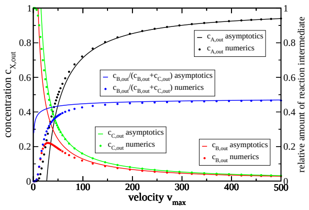

Fig. 4: *Species concentration and relative amount of intermediate products of a multistep catalytic surface reaction at the outlet of a flow cell depending on inflow velocity; see [5]*

Mathematical and numerical modeling of coupled flow processes in electrochemical devices

Electrochemical energy storage systems like batteries and fuel cells play a central role for energy supply. Mathematical and numerical modeling contributes to the understanding of these devices and potentially allows to improve and optimize them. Based on compatible discretization approaches, see the Scientific Highlights article on page 40, the group focuses on the macroscopic modeling of thin layer flow cells, which are electrochemical cells that allow to investigate separate processes in a simpler and better controlled experimental setting. Qualitative [5] and quantitative comparisons to measurements undertaken by experimental groups have been successful; see Figure 4. Together with the Research Group *Thermodynamic Modeling and Analysis of Phase Transitions*, the group organized the workshop "Mathematical Modeling and Experimental Investigation of Electrochemical Processes in Energy Storage Systems" (MODELCHEM 2011), which brought together a significant number of researchers active in the modeling of batteries and fuel cells.

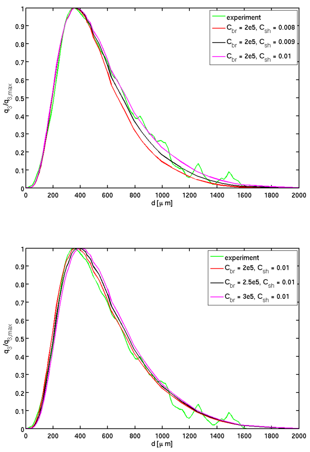

Fig. 5: *Example of the calibration of model parameters in the aggregation kernel for the synthesis of urea; top: parameter with respect to shear-induced aggregation; bottom parameter with respect to Brownian motion induced aggregation*

Numerical simulations of population balance systems

Population balance systems model particulate flows where not the behavior of individual particles is of interest but the behavior of the particles in the mean. The mean behavior is modeled by an equation for the particle size distribution (PSD).

A main achievement in 2011 was the completion of the incorporation of aggregation (or coalescence) of particles into the model. This work was done in collaboration with the group of Wolfgang Hackbusch (Max Planck Institute for Mathematics in the Sciences, Leipzig). An important issue in the numerical simulations is the calibration of unknown model parameters in the aggregation kernel. This calibration was performed for a model of the synthesis of urea by comparing the results of numerical simulations with experimental data. A trial and error procedure was used, which is, however, rather inefficient. Since the appearance of unknown parameters can be expected often in models from applications, more efficient approaches have to be developed. This aspect is the main motivation for the study of model order reduction methods, like POD, for coupled flow problems.

The equation for the PSD is a scalar convection-dominated equation. Based on the assessment of discretizations for this type of equation from [3], an ENO finite difference method with TVD Runge–Kutta scheme is now used as standard discretization for this equation.

Optimization and statistical fleet analysis for gas turbines

The process simulator BOP provides different modes for steady-state, transient, Monte Carlo, correction-curve, and homotopy simulations to treat large-scale systems of differential-algebraic equations arising in process simulation problems. Besides these so-called *internal simulation* *modes*, some simulation add-ons have been added to BOP. Two of them are the Optimization Add-On and the Statistical Fleet Analysis Add-On. It is common to both add-ons that they use multiple simulation runs of BOP internal modes.

The Optimization Add-On, called *MSO (Modified least-Squares Optimization)* mode, allows for the prediction of input parameters of a process while matching output parameters within certain tolerance bounds. The existing application, implemented as a Levenberg–Marquardt algorithm, was extended to optimization problems that rely on multiple simulations of one process example, e. g., using different input parameters. In this way, the same output variables of different simulations can be "drawn nearer" to each other without exact knowledge of the "real values". A main application area consists in the evaluation of measurement errors and the validation of relevant process parameters. The MSO application makes it possible to define settings for multiple steady-state simulations and to formulate a common least-squares optimization problem, e. g., from given tolerance ranges for input variables. Within an iterative trust-region search, Jacobian information from multiple steady-state simulations is used.

In an industrial application at Alstom Power Ltd., the BOP MSO mode has shown promising results for the optimization of heat balance data for gas turbine models with respect to some uncertain measurements.

The second BOP add-on, called *Statistical Fleet Analysis Add-On*, concerns a statistical analysis tool to determine the scatter of measurement data for comparable process models, e. g., the *fleet scatter* of worldwide operating gas turbines. The aim of this project consists in improving the accuracy of common performance guarantees for all these models. The data must be evaluated with respect to a reference curve or a reference point. The former problem is thus a subject of regression analysis (mixed-effects model), whereas the latter uses the concept of the statistical depth. In the reference-point case, the ideal data would collapse to the reference point. Instead, the real data are represented by a point cloud, and each point in the plane is assigned a depth with respect to the given point cloud. Points outside have depth zero, and points within the cloud have a depth according to Tukey's half-space depth. In the bivariate case, the deepest point, having maximal depth, can be computed exactly and may be considered as representing the center of the cloud. Additionally, the polygonal contour is constructed, which may be considered as a confidence region (called *iso-depth contour*) for the point cloud. If the reference point is inside the iso-depth contour, then it represents the data given at such confidence level.

The new version BOP2.8, including the new add-ons as well as other improvements, will be released in March 2012.

Evolution model for phase transformations in steel

In heat treatment simulations, it is of great importance to model the time-dependent behavior of the steel phases with a rate equation. For the special case of isothermal transformation, a frequently used phenomenological ansatz, describing the decomposition of austenite into one phase $y \in [0,1]$ of ferrite, pearlite, or bainite, is

$$y'(t) = (a + y(t))^r (y_{eq} - y(t))^s g \,, \quad y(0) = y_0 \,, \quad t > 0 .$$

It is known that the model case $y(0) = y_0$, $a = 0$, leads to a thermomechanical inconsistency for general processes. The other model case of interest, $y_0 = 0$, $a > 0$, tries to fix this problem. In contrary to calculating the best-fitting parameters r, s, g, a, y_0, the focus of the investigations in [8] lies on the following question: How well is it possible to determine the parameters of a model *in principle*? Basically, the phase transformation should fulfill the material data conditions obtained from an isothermal transformation diagram. This question leads to the inverse problem that the data condition holds for a solution y.

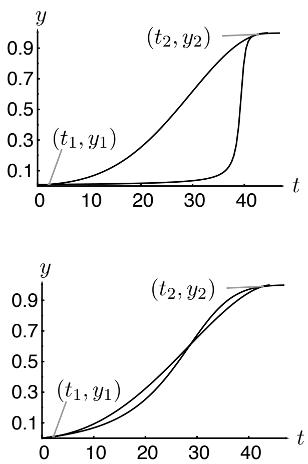

***Fig. 6:** Possible range of transition characteristics at an isothermal temperature for the model case $y_0 > 0$ (top) and for the model case $a > 0$ (bottom)*

The results shown in [8] are as follows. Only the first model case $y_0 > 0$ is *in principle* able to match all starting and end phase fractions of the isothermals exactly. Furthermore, if a transformation curve exists for given material data, then it is not unique. But it is possible for both models to identify a set of independent parameters, which are free of choice in a well-defined range. This range leads to an array of transformation curves, which may be interpreted as a range of possible transformation characteristics; see the schematic plots in Figure 6. Moreover, the independent parameters have clear geometricals meanings, and in their range, the existence of a unique solution is ensured. However, for the reliable simulation of themomechanical processes, it is highly desirable to propose a new model without the drawbacks of the two models studied.

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4.4 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.

In 2011, the group continued its participation in the DFG Priority Programs SPP 1180 and SPP 1204, respectively. It is actively engaged in the DFG Research Center MATHEON with four projects (B20, C7, C11, and C30) and it runs the DFG Individual Grant project "Direct and inverse scattering problems for elastic waves". The group coordinates two collaborative projects with scientific and industrial partners within the BMBF Program "Mathematics for Innovations in Industry and Services" and by the Central Innovation Program for small and medium-sized enterprises ZIM, respectively. In addition, it is involved in three privately funded projects with industrial partners. For the projects, see also pages 94 ff.

Three of the research group's students successfully defended their Ph.D. theses and took up positions in industry. Another highlight was the organization of the 25th IFIP TC 7 Conference on System Modelling and Optimization together with Fredi Tröltzsch (Technische Universität Berlin). It is part of a biennial conference series with preceding conferences in Buenos Aires (2009), Cracow (2007), and Turin (2005). With 315 participants from 37 countries, 288 lectures, the majority of them delivered in 67 minisymposia and 8 contributed sessions, the conference became a great success. It showed the attractiveness of the IFIP TC 7 concept linking research in abstract mathematical optimization and control theory and building a bridge to numerical methods and applications in various fields.

In the following, scientific achievements of the research group in 2011 are detailed.

Optimization and optimal control

Fig. 1: *Compressor station in a gas network*

The theory, numerics, and applications of nonsmooth and stochastic optimization continue to be a main area of research in the group. These activities are closely related to the MATHEON projects C7 "Stochastic optimization models for electricity production in liberalized markets" and B20 "Optimization of gas transport", as well as to an industry project on gas network optimization. Substantial progress was made in broadening the class of probabilistically constrained optimization problems amenable to numerical solution. This progress concerned, in particular, polyhedral constraints with Gaussian coefficients. The investigations of the ISO (independent system operator) electricity spot market model (within C7) were completed by a detailed analysis of the underlying equilibrium problem with equilibrium constraints (EPEC) provided in [4]. Here, structural conditions of the model were identified, which ensure the so-called *calmness* of a perturbation mapping, a key for deriving first-order optimality conditions. The focus of this topic now shifted to European power market models like the European Energy Exchange (EEX) and the European Power Exchange

(EPEX). Further work in nonsmooth optimization was devoted to equilibrium constraints with non-unique multipliers and to the investigation of structural properties (e. g., eccentricity) of convex cones.

Within the MATHEON project C30 "Automatic reconfiguration of robotic welding cells", the focus in 2011 was on computing the fastest collision-free trajectory of a robot moving from an initial position to a given final state [2]. An active-set strategy based on backface culling was developed. The main idea is to apply anti-collision constraints only when the robot is close enough to the obstacle and only between the faces of the robot and the obstacle that are facing each other. The new approach results in four times faster computing times and a drastic reduction of the problem size.

In a joint work with Joachim Rehberg (Research Group *Partial Differential Equations*), optimal control problems with semilinear parabolic partial differential equations and pointwise state and control constraints were discussed. The underlying parabolic equations are considered with the help of the concept of maximal parabolic regularity. By means of this concept, it was possible to extend known results for second-order sufficient optimality conditions for this type of problems also to two- and three-dimensional problems [1].

In the framework of the DFG Priority Program SPP 1204, an optimal control problem in the cooling section after hot-rolling of multiphase steels was considered, where the time-dependent water amount serves as control variable. The optimal control problem is governed by a nonlinear coupled system of the heat equation and phase transition equations. The problem was analyzed regarding the existence of (local) optimal solutions and first- and second-order optimality conditions. Furthermore, a reduced sequential quadratic programming method was applied to the problem in order to solve it numerically.

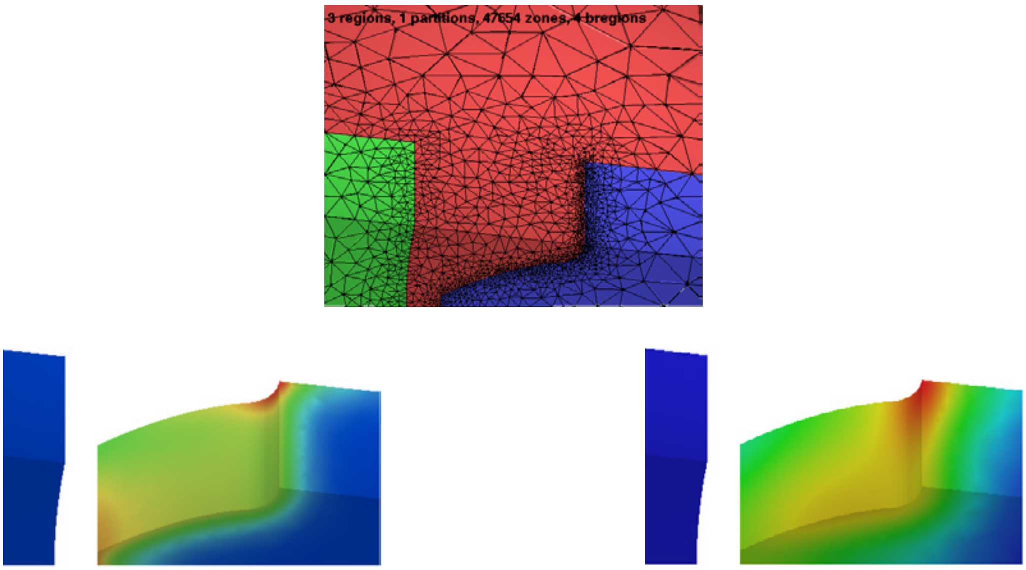

Fig. 2: *Adaptive grid resolving eddy current region (top); temperature profile at high frequency showing heating of tooth tip (bottom left); temperature profile at medium frequency showing heating of tooth base (bottom right)*

In July 2010, the project "Modeling, simulation and optimization of multifrequency induction hardening" (MeFreSim) within the BMBF Program "Mathematics for Innovations in Industry and Services" started. After implementation of lowest-order edge elements to solve Maxwell's equation, the focus in 2011 was to extend them to hierarchical basis functions for H(curl) of arbitrary polynomial degree. Furthermore, a residual error estimator has been implemented that allows for the use of adaptive grid refinement; cf. Figure 2.

Inverse problems

Diffraction phenomena for elastic waves propagating in unbounded periodic and non-periodic structures have many applications in geophysics and seismology. For instance, the problem of elastic pulse transmission and reflection through the earth is fundamental to the investigation of earthquakes and the utility of controlled explosions in search of oil and ore bodies. Extending previous work on elastic diffraction gratings within the DFG Individual Grant project "Direct and inverse scattering problems for elastic waves", a novel variational approach for the elastic scattering by rough surfaces was developed, leading to new existence and uniqueness results for the direct scattering problem at arbitrary frequency [3].

To reconstruct the profile of a two-dimensional elastic diffraction grating from near- and far-field data, this highly ill-posed problem was reformulated as a nonlinear optimization problem for the Dirichlet boundary value problem of the Navier equation. The optimization method combined with Tikhonov regularization was applied to smooth and piecewise linear gratings, and satisfactory numerical reconstructions from exact and noisy data were obtained. Moreover, new global uniqueness results for the inverse scattering of time-harmonic plane elastic waves by a biperiodic diffraction grating were established. In particular, all unidentifiable polyhedral grating profiles that correspond to only one given incident elastic field could be completely classified.

For the scatterometric measurement of photolithographic masks, the work on the corresponding inverse problems reconstructing periodic surface structures was continued. An algorithm for the reconstruction of biperiodic gratings from scatterometry data was developed. In particular, this algorithm computes the parameters of a symmetric biperiodic contact hole structure with layered boundary and of a symmetric biperiodic array of layered frustums of pyramids. The set of free parameters to be reconstructed can be reduced by fixing possible dependencies.

For the gradient-based optimization in the above algorithm, the formula for the shape derivative was further developed. In the two-dimensional case the approach leads to unbounded terms in the formula, which can be avoided using classical techniques for the magnetic fields and substituting the magnetic field by the electric one. This formula was further simplified so that all ingredients are entities obtained directly by the finite element method (FEM) for the electric field equation. Together with the convergence of the FEM, the convergence of the shape derivatives is guaranteed; cf. [5]. The formula was implemented to compute the Jacobian matrix for the Gauss–Newton iteration of the reconstruction algorithm.

The program package `DiPoG` for the two-dimensional case was extended. The new version admits the scatterometric reconstruction of the widths in the underlying multi-layer system by a least-squares approach and of the noise levels by a maximum-likelihood method. Finally, based on a $\chi 2$-test, the estimates for the uncertainties of the reconstructed data were improved. Moreover, the impact of line-edge and line-width roughness on the reconstruction of masks was simulated. A simplified model, assuming low-frequency corrugations, can be treated as proposed by Akiko Kato and Frank Scholze (Physikalisch-Technische Bundesanstalt, Berlin) by incorporating the Debye–Waller factor to correct the scatterometry input data.

The integral equation solver for conical diffraction was extended, especially the algorithms for multi-profile gratings, where the interfaces between adjacent grating materials cannot be separated by horizontal planes. Different operator recursion algorithms, which can be adapted to integral methods, were investigated and numerically tested. This research led to an improved version of Maystre's approach introduced originally for in-plane diffraction, together with necessary and sufficient conditions of its applicability. It is planned to implement these new algorithms into an optical modeling software tool. The integral equation solver for gratings with separated interfaces was improved to treat also technologically relevant two-dimensional photonic crystal gratings with different periods and crystals. In [6], the vital role of conical diffraction compared to the in-plane case as well as of the incidence polarization were demonstrated in many situations. Figure 3 compares some diffraction properties of non-absorbing photonic crystal gratings with dielectric rods. Besides the filling ratio, refractive index, and polarization, the off-plane diffraction gives an additional control parameter, which significantly influences existing photonic band gaps.

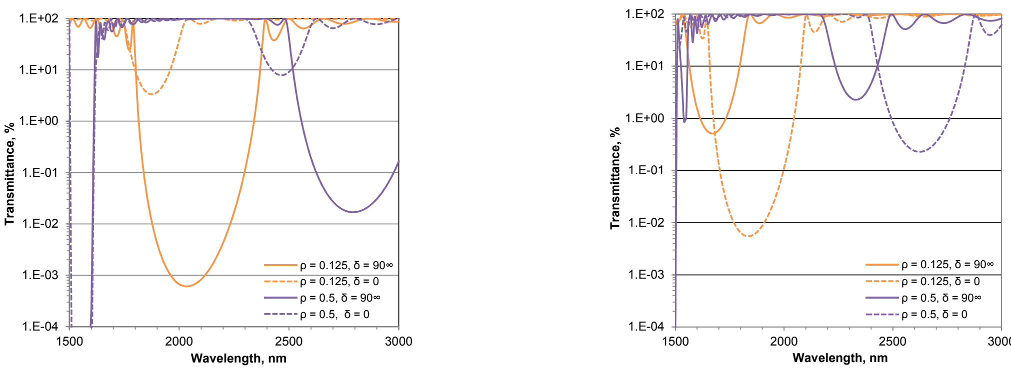

Fig. 3: *Calculated transmission spectra of a $d = 1\,\mu$m grating with dielectric circular rods with filling ratio ρ embedded in vacuum are plotted vs. wavelength of incidence radiation with polarization angle δ and $\phi = 0$ (classical diffraction, left), and $\phi = 30^\circ$ (conical diffraction, right)*

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4.5 Research Group 5 "Interacting Random Systems"

Having finally filled all the positions at the end of 2010, the research group took up its activities with fresh forces. Two more researchers completed the team, funded by the Weierstrass Postdoctoral Fellowship program and by the Alexander von Humboldt foundation, respectively. This personnel reinforcement enabled a host of successful work on a number of topics, like random walks in random environment, branching processes, and the subjects described below.

The DFG Research Unit FOR 718 *Analysis and Stochastics in Complex Physical Systems*, led by the head of the research group, Wolfgang König, 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 in 2011. On the occasion of two international workshops held in 2010 at Technische Universität Berlin, a prestigous Festschrift was edited by Wolfgang König in 2011, which will appear in a new Springer series in 2012.

Further activities of group members in 2011 included an invited plenary lecture at the 8th International Conference on Large-Scale Scientific Computations in Sozopol, Bulgaria, and the coordination of the Summer School of the Berlin Mathematical School on "Random Motions and Random Graphs". The Center for Mathematics and Science Education and Hands-on Museum "INSPIRATA", located in Leipzig and chaired by Wolfgang König, received two important and widely recognized prizes, the title "Idea for the Federal Republic of Learning", issued by the initiative "Germany — Land of Ideas", and the presentation, in the INSPIRATA rooms, of the exhibition MATHEMA, which was running with extraordinary success in the Deutsches Technikmuseum in the Year of Mathematics, 2008.

Stochastic models for coagulation-advection problems

Stochastic models of particle formation and growth have been successfully used in several areas of chemical engineering in recent years. The formation of soot particles in combustion systems is a highly complex process, which calls for detailed modeling of the resulting soot particle populations (see Figure 1). The stochastic approach allows for arbitrarily complex models of individual particles to be included with little additional impact on computation times. A common tool for the mathematical treatment of the subject are nonlinear partial integro-differential equations, which are closely related to stochastic interacting particle models.

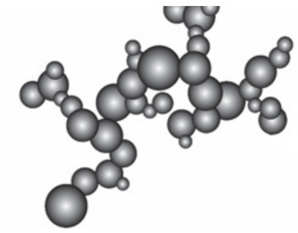

Fig. 1: *Schematic of a soot particle*

Several new results were obtained in collaboration with the Department of Chemical Engineering and Biotechnology (University of Cambridge, UK). A class of stochastic algorithms for the numerical treatment of population balance equations was introduced in [5]. The algorithms are based on systems of weighted particles, in which coagulation events are modeled using a weight transfer that keeps the number of computational particles constant. The weighting mechanisms are designed in such a way that physical processes changing individual particles (such as growth, or other surface reactions) can be conveniently treated by the algorithms. A spatially resolved stochastic weighted particle method for coagulation-advection problems with inception was presented in [6]. Convergence to a deterministic limit is studied. Numerical experiments show the method to be robust and confirm the convergence properties. The robustness of the weighted particle method is shown to contrast with two Direct Simulation Algorithms which develop instabilities.

Connectivity in mobile ad-hoc networks

Mobile ad-hoc networks represent a dynamic research area in telecommunications science. In contrast to standard telecommunications networks, where immobile devices (antenna, satellite) connect the users, in an ad-hoc network, the devices carried by the users play the role of these antennas. Two participants can communicate with each other at a given time if they are connected by a chain of participants along which the respective connection lengths are shorter than a given radius, the *connection range*. Hence, the system is a variant of a continuum percolation system. The main questions are about the time laps over which two given participants of the system are connected, the size of the largest connected component in the system, the time that it takes a message to be delivered, and more.

An important aspect of the model is the random movement of the individual users. For a realistic modeling, the *random waypoint model*, rather than Brownian motion or standard random walks, is considered. However, this model has not been the object of mathematical study yet, and most of the existing literature is based on numerics and heuristics only.

In the group, the thermodynamic limit of a mobile ad-hoc network is considered, where the system is large and the area of the domain considered is of the order of the number of participants. Using tools from ergodic theory, percolation theory, renewal theory, and 0-1 laws, explicit formulas were obtained for the average time that two given participants can communicate with each other, conditional on their trajectories or unconditional. Further work described the long-time behavior of this quantity in terms of a law of large numbers and the probability of deviations from the usual behavior in terms of a large-deviation principle.

Large deviations for the local times of a random walk among random conductances

Many problems in statistical physics, such as mass transport or heat distribution in homogeneous media, have been known for a long time to be accessible by probabilistic methods, in particular, by random walk models. With regard to most of these applications, it seems more realistic to model particle diffusion and heat distribution dynamics rather in an inhomogeneous (i. e., randomly perturbed) medium. A promising model in this respect is the *random conductance model*, which assigns a random positive weight to each edge of the discrete lattice, which measures the strength of the mass flow along this edge.

The study of local time asymptotics is a basic step towards an understanding of the model. One of the main motivations is the *parabolic Anderson model*, that is, the Cauchy problem for the heat equation, with random conductances and an i.i.d. random potential. Via the Feynman–Kac formula, the total mass in that model is described in terms of the local times of the underlying random walk. As a fundamental pre-step, the group analyzes the behavior of the local times in boxes in the long-time limit.

Assuming that the conductances may assume arbitrarily small values, in [4] a *large deviation principle* (LDP) in fixed boxes was derived. The scale and the rate function of the LDP are explicit in terms of the model parameters. In this setting, the annealed (i. e., when averaged over the conductances and the walk) behavior of the local times comes from a combined strategy of the conductances and the random walk. This strategy is that the conductances assume small time-dependent values and the walker realizes very large time-dependent holding times and/or trajectories that do not leave the region.

Interacting particle systems in continuous configuration space

The microscopic theory of phase transitions rests on the formalism of statistical physics, as introduced by Boltzmann and Gibbs. In applications, ranging from chemical engineering to meteorology, the formalism enters the derivation of, e. g., equations of state, which can then be used in computer simulations.

From a more fundamental point of view, the question arises whether the existence of phase transitions can be deduced from the microscopic statistical model. While this question has been answered positively in a wide variety of discrete models, little is known about continuous systems. One intuitive picture is the theory of Frenkel and Band, who "... pointed out the value of regarding the imperfection and condensation of real gases as association equilibria of molecules into physical clusters of various sizes, [... condensation is] supposed to be due to sudden appearance of clusters of macroscopic size" (Stillinger, J. Chem. Phys. 38, 1963).

Motivated by this geometric picture, the research group studies the formation of *clusters*, groups of particles close to each other. Particles live in continuous configuration space and interact via a finite-range Lennard–Jones-type potential. Their distribution is given by a canonical Gibbs measure in a finite volume. In [1], an abstract large deviation principle was proved for the cluster size distribution in the thermodynamic limit. In a certain low-temperature, low-density limit, the rate function was shown to Gamma-converge to an explicitly known affine rate function. This fact has consequences for the limit behavior of the cluster size distribution, in particular, for the existence of a transition from small to large cluster sizes. The Gamma-convergence is best understood by showing that the cluster size distribution behaves like a random partition model with multiplicative weights, known in physics as an *ideal mixture*. In [3], estimates were proved on the difference between the original rate function and the explicit rate function associated with the approximate model. Furthermore, the Mayer and virial expansions of the pressure were investigated in [2], and it was shown that their low-temperature behavior is consistent with the results from [3] and [1]. Physical interpretations for the Mayer and virial series' radii of convergence were proposed and results on where to look for gas-solid phase transitions, in the spirit of the Lee–Yang theorem for lattice gases, were deduced.

Metastability in statistical mechanics

The out-of-equilibrium dynamics of some complex disordered systems exhibits very interesting phenomena, such as aging, rejuvenation, and memory effects. One such class of systems where these phenomena were observed experimentally is the spin glasses. Aging, which roughly means that the system has age dependent decorrelation properties, was explained on a phenomenological level by Bouchaud's trap model of random energy type. Only recently, the aging displayed in this model was extended to a wide range of spin glasses for various time scales. However, this model is not enough to explain aging for some important spin glass models or the memory effects and rejuvenation. The reason for this insufficiency is that in the thermodynamic limit the energies of spin glasses are organized hierarchically, while Bouchaud's trap model does not contain such a structure.

With the goal of understanding the effects of a hierarchical structure on the dynamics, the group introduced generalizations of the above models, where the energies governing the dynamics are given through a hierarchical structure induced by a general class of trees. Next, the right decorrelation functions to study in order to best capture the effects of this hierarchical structure on aging were identified. Then, using the tools from point processes, it was proved that the system ages with different limiting aging functions depending on the time scale of the observation. Currently, the group is working on developing necessary tools to prove that this model exhibits memory effects and rejuvenation and on extending its results to a more general class of spin glass models.

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4.6 Research Group 6 "Stochastic Algorithms and Nonparametric Statistics"

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

The research group has reached a leading position with important mathematical contributions and the development of statistical software. Part of the research is carried out within the two MATHEON projects F10 and E5 and the SFB 649 projects B5 and B7; see page 95. The group participated in two projects, with the German Diabetes Center Düsseldorf (DDZ) and with the Potsdam Institute for Climate Impact Research (PIK), within the *Pact for Research and Innovation* (see page 96). Members of the group were involved in several industrial contracts. The existing cooperation with HSH Nordbank on pricing and calibration of different financial instruments was continued. The group also participates in a project with Alstom (Switzerland) Ltd., on "Gas turbine process simulation". The contribution concentrates on general statistical modeling and sensitivity analysis using Monte Carlo methods.

Scientific highlights achieved by the research group in 2011 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 regularization and estimation in inverse problems, dimension reduction, multiple testing, signal detection, feature identification, and adaptive smoothing in various applications.

Highlights 2011:

- Mega Grant awarded by Russian government to Vladimir Spokoiny
- Workshop on Statistics and Neuroimaging, WIAS, November 23–25, 2011
- Special volume "Magnetic Resonance Imaging in R" edited by Karsten Tabelow and Brandon Whitcher (London) appeared in Journal of Statistical Software in October 2011. http://www.jstatsoft.org/v44

Modern applications raise new challenges to statistical theory. The main issues to be addressed are the high dimension of the parameter space and robustness against possible model misspecification. The classical asymptotic parametric theory fails to cover these issues. The group is actively working on developing novel approaches and methods that allow for high-dimensional parameters and are applicable even for incorrectly specified models. The proposed approach extends Le Cam's famous *local asymptotic normality* theory and can be applied in a unified way for obtaining the nonasymptotic analogs of the classical results like Wilks's, Fisher's, and Bernstein–von Mises's theorems; see [5].

A monograph on modern statistical parametric theory is in preparation.

Neuroimaging is a rapidly developing area that is driven by advances in Magnetic Resonance (MR) technology and the combination of many different disciplines like mathematics, physics, medicine, psychology, neurology, and computer sciences. Problems formulated in the neurosciences include the identification of gray matter areas that are related to the functional activity of the brain (fMRI), a description of the anisotropy of white matter fiber structures (dMRI), or the identification of fiber bundles connecting different areas (connectivity analysis).

Clinical applications focus on diagnostics based on within-group variability, between-group differences, and changes in time series of derived quantities. Presurgical planning depends on the identification of abnormalities in the brain.

All these problems and applications create a need for appropriate statistical modeling and new data analysis methods. Special challenges are created by amplified noise due to increasing image resolution.

Research on these problems is carried out, e. g., within the MATHEON project F10 "Image and signal processing in the biomedical sciences: Diffusion weighted imaging — Modeling and beyond". In 2011, this research led to a new method for orientation density estimation in diffusion MRI. The proposed model is physically motivated and enables a description of partial volume effects that are hidden in the traditional diffusion tensor based analysis; see [6].

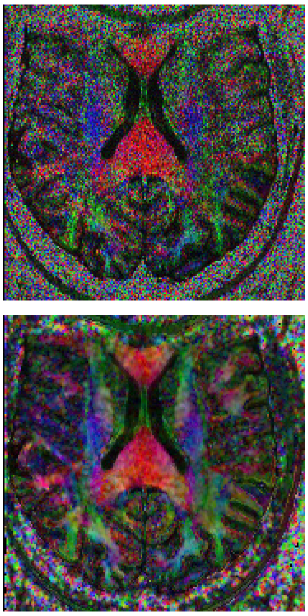

Fig. 1: *Position-orientation adaptive smoothing (POAS) of an ultra-high resolution dMRI data set. Upper: estimated color-coded FA map without smoothing. Lower: result using 12 steps of POAS.*

A new innovative approach was proposed for efficient noise reduction in imaging data from diffusion MRI. The method, position-orientation adaptive smoothing (POAS),employs an embedding of the measurement space into a space with defined metric and group operations, in this case the Lie group of three-dimensional Euclidean motion SE(3). Adaptation to the unknown structure is achieved by an iterative strategy of pairwise comparisons of preliminary estimates. In contrast to preliminary proposals, the method does not employ any specific model for the data. Figure 1 provides an estimated color-coded fractional anisotropy (FA) map without and with POAS smoothing for an ultra-high resolution ($800\,\mu m$ isotropic resolution, 60 gradient directions, data kindly provided by Robin Heidemann (Max Planck Institute (MPI) for Human Cognitive and Brain Sciences, Leipzig)); see [2] for details.

Research on these topics is carried out in cooperation with partners from Weill Medical College, New York, USA, the Universitätsklinikum Münster, the Bernstein Center of Computational Neuroscience (BCCN) Berlin, and the MPI for Human Cognitive and Brain Sciences, Leipzig. Statistical methods for imaging and neuroscience applications were implemented in 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)*.

A workshop on "Statistics and Neuroimaging", organized at WIAS, brought together internationally recognized experts with backgrounds in mathematics, physics, neuroscience, statistics, medicine, and psychology for a very fruitful exchange and discussion on state-of-the-art procedures and current challenges.

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 2011:

- Co-organization of the workshop "Asymptotic Expansions in Applied Analysis and Stochastics", WIAS, October 10–11, 2011
- Ronnie Loeffen accepted a W2-professorship offer of the University of Manchester

The research on general multiple stopping problems in the context of complex structured (swing) options in electricity markets that involve volume constraints and refraction periods was completed. Further details and references can be found in the Scientific Highlights article on page 20 in this report.

The regression-based dual valuation algorithm for American options developed in the preceding year was further improved. Moreover, this fast non-nested Monte Carlo algorithm, which doesn't need any "input" approximation to the problem under consideration, was successfully extended for standard multiple stopping problems and in a recent study applied to the pricing of flexible caps [1].

In the area of interest-rate modeling, the focus was this year on Lévy-driven LIBOR models. While these jump models with infinite activity are quite flexible from an economics point of view, their simulation was known to be problematic due to a complicated structure of the drift term. In this respect, new log-Lévy LIBOR approximations were constructed that resolve this problem and allow for fast Monte Carlo simulation [4].

In the context of Monte Carlo simulation of European options, Michael B. Giles (Oxford) initiated in 2008 a new trend called *multilevel Monte Carlo* by constructing a "telescoping estimator" due to different levels of time discretization of the stochastic differential equation. The idea of Giles was exploited in a completely different context in order to construct a multilevel version of the Andersen–Broadie dual algorithm for American options. In this new algorithm, the multilevel idea is applied to the number of sub-simulations rather than SDE time steps. As a result, the AB complexity of ϵ^{-3} reduces to $\epsilon^{-2}\ln^2\epsilon$, which is virtually the complexity of non-nested simulation [3]. As a next project in this area, the development of a multilevel version of the Kolodko–Schoenmakers policy iteration was started.

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4.7 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

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 modeling and analysis of transformations and storage of energy have become an important issue.

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 producing mechanical stresses, the appearance of precipitates in crystals leading to lattice deformations, nonlocal radiation fields interacting with nonconvective heat conduction, and long-range energetic as well as entropic interactions leading to nonlocal PDEs.

Highlights

1. In 2011, Wolfgang Dreyer successfully participated in the competition procedure of the Leibniz Association in the Pact for Research and Innovation. The proposed project “Mathematical models for phase transitions in lithium-ion batteries” will be funded with 616,200 Euros for three years. The funding will be used to establish a new Leibniz group, where a new model covering slow and fast charging regimes including mechanics and the transfer problem between the battery electrodes and the electrolyte will be studied. The chemical essentials of the new many-particle model are described in the paper “The thermodynamic origin of hysteresis in insertion batteries” [6], the corresponding mathematical model and numerical simulations are treated in the article “Hysteresis and phase transition in many-particle storage systems” [7], and the mathematical analysis is found in the preprint “Blow-up versus boundedness in a nonlocal and nonlinear Fokker–Planck equation” [2].

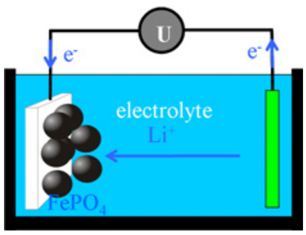


Fig. 1: *The many-particle electrode of a lithium-ion battery*

2. In 2011, the investigation of a new model for diffusive phase segregation due to Paolo Podio-Guidugli (Rome) was successfully continued. The model leads to a new class of phase field equations of the form

$$(\varepsilon + 2\rho)\,\mu_t \,+\, \rho_t\,\mu \,-\, \Delta\mu \;=\; 0\,, \tag{1}$$

$$\delta\rho_t \,-\, \Delta\rho \,+\, f'(\rho) \;=\; \mu\,. \tag{2}$$

Here, ρ is an order parameter, μ is the chemical potential, and ε and δ are positive constants.

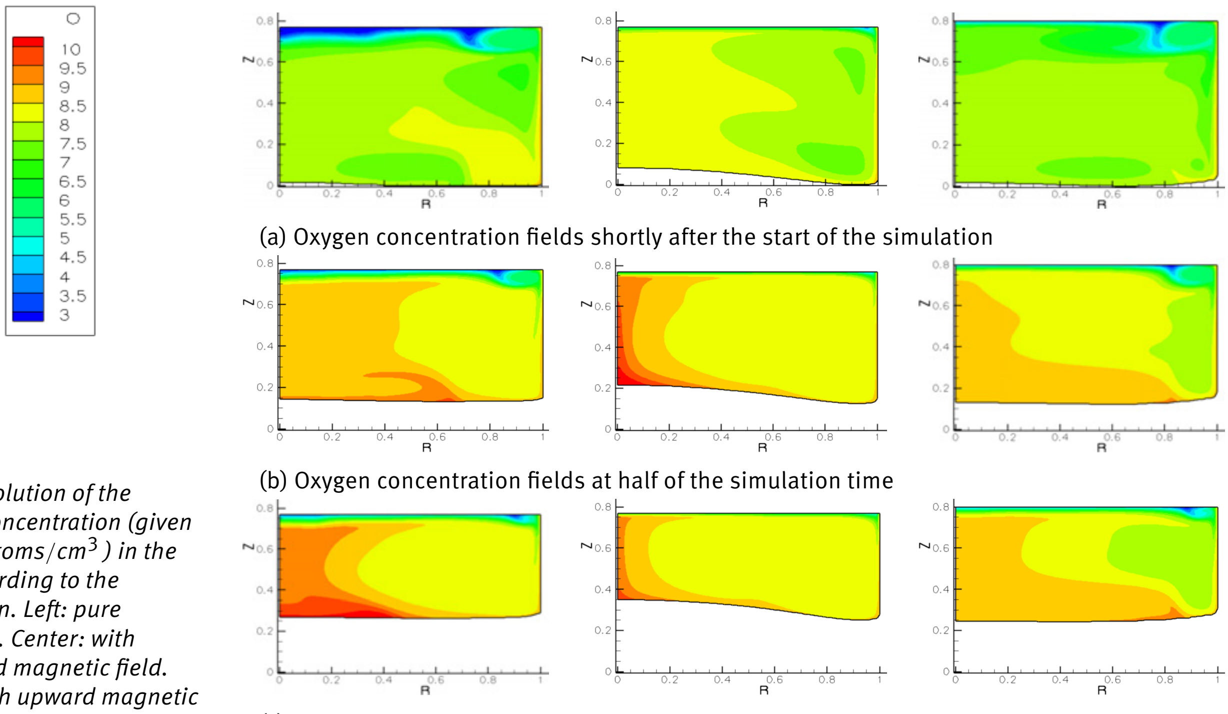
The coarse-grain free energy f is typically of the form $f = f_1 + f_2$, where f_2 is smooth and $f_1(\rho) = \rho\,\ln(\rho) + (1-\rho)\,\ln(1-\rho)$. The system (1), (2) is a highly nonlinearly coupled system of singular partial differential equations whose analysis requires delicate estimates and deep analytic tools. In particular, it is necessary to prove that the unknowns μ and ρ obey the both physically and mathematically relevant constraints that μ be nonnegative and bounded and $0 < \rho < 1$.

In [3], well-posedness, regularity, and the asmptotic behavior as $t \to +\infty$ was treated, and in [4], distributed optimal control problems for system (1), (2) were studied. In addition, a rigorous asymptotic analysis of the system as $\varepsilon \searrow 0$ was performed in a forthcoming paper.

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 example may give some illustration.

The interdisciplinary project AVANT*SOLAR* addresses the optimization of crystal growth processes that produce extremely large silicon crystals of rectangular shape. It is funded by industrial partners and the "Zukunftsfonds" of the Federal State of Berlin. In June 2011, the project ended successfully.



(a) Oxygen concentration fields shortly after the start of the simulation

(b) Oxygen concentration fields at half of the simulation time

(c) Oxygen concentration fields at the end of the simulation time

Fig. 2: *Evolution of the oxygen concentration (given in 10^{17} atoms/cm^3) in the melt according to the simulation. Left: pure buoyancy. Center: with downward magnetic field. Right: with upward magnetic field*

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 and, in particular, in the vicinity of the liquid-crystal interface; see [1]. To this end, the coupled Navier–Stokes–Fourier diffusion system was solved. The computation relied on data from another project partner concerning position and temperature of the melt-crystal interface.

Funded under Priority Programs of the German Research Foundation

Dirk Peschka and Barbara Wagner participate 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 study “Stationary solutions for two-layer lubrication equations” [5]. Here the stationary flow of thin liquid bilayers is described by an energetic formulation of gradient flow structure. Γ-convergence techniques are used to derive the corresponding sharp-interface model.

DFG-CNRS research group

Within the framework of a German-French research group on liquid-vapor flow, Wolfgang Dreyer and Christiane Kraus from the Leibniz Group *Modeling of Damage Processes* jointly guided an interdisciplinary project on diffuse interface models that include temperature variations and phase transitions between liquid and vapor. The industrial context of the project concerns cavitation bubbles in the cooling system of nuclear plants and, in particular, near to walls. In 2011, a new model describing the evolution of two incompressible fluids with phase transition was proposed and exploited. The model consists of a PDE system for three variables: (volumetric) phase fraction φ, (barycentric) velocity $\mathbf{v}$, and a Lagrange multiplier λ that takes care of the kinematic condition of incompressibility.

$$
\begin{aligned}
&\partial_t\varphi + \operatorname{div}(\mathbf{v}\varphi) = c_+\big(m_{\,\mathrm{j}}\Delta - m_{\,\mathrm{r}}\big)(c_+\mu(\varphi) + c_-\lambda),\\
&\rho(\varphi)(\partial_t\mathbf{v} + (\mathbf{v}\cdot\nabla)\mathbf{v}) + \nabla p(\varphi) + \nabla\lambda\\
&\qquad\qquad = \nabla(\eta(\varphi)\operatorname{div}\mathbf{v}) + \operatorname{div}(\hat{\eta}(\varphi)(\nabla\mathbf{v} + \nabla\mathbf{v}^T)) + \gamma\,\varphi\nabla\Delta\varphi,\\
&\operatorname{div}\mathbf{v} = c_-\big(m_{\,\mathrm{j}}\Delta - m_{\mathrm{r}}\big)(c_+\mu(\varphi) + c_-\lambda),
\end{aligned}
\tag{NS-CH}
$$

where the chemical potential μ and the non-monotone pressure p are derived from a double-well energy function according to

$$
\mu(\varphi) = W'(\varphi) - \gamma\,\Delta\varphi, \qquad \text{and} \qquad p(\varphi) = \varphi W'(\varphi) - W(\varphi). \tag{3}
$$

Jointly with groups from Freiburg and Stuttgart, headed by Dietmar Kröner and Christian Rhode, respectively, Gonca L. Aki studied various sharp limits of the system leading to the Euler regime as well as to the Navier–Stokes regime. In particular, generalized versions of the Young–Laplace law and the Gibbs–Thomson law could be derived.

MATHEON projects

The research group contributed with four projects to 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"

Among the objectives of project C10, guided by Barbara Wagner, is a study of the dynamics of suspended particles in liquids [2] by Dirk Peschka. A related problem, and a very old one, concerns the decomposition of a liquid droplet in contact with a liquid layer due to shear forces. This phenomenon is modeled by two coupled Cahn–Hilliard equations with non-constant mobilities, which degenerate for certain values of the variables.

Fig. 3: *Left: A droplet of glycerol flows down an inclined plane that is wetted by a liquid. The droplet size is in an unstable regime where shear forces lead to a decomposition into smaller droplets. Right: The experimental phenomenon is encoded in a system of coupled PDEs that likewise exhibits the decomposition.*

Ph.D. students

Wolfgang Dreyer, Jürgen Sprekels, and Barbara Wagner, jointly with other partners, guide and supervise six 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.

The 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, chemical reactions, and mechanical stresses, (ii) liquid flow in magnetic fields with heat conduction, (iii) nucleation and collapse of bubbles within flow patterns. Thus, there arise involved initial-boundary value problems for nonlinear coupled systems of partial differential equations.

Miscellaneous

Barbara Wagner, deputy head of the research group, accepted a call to a professorship in Mathematical Models of Photovoltaics at the Technische Universität Berlin.

In November 2011, the research group, jointly with Jürgen Fuhrmann from the Research Group *Numerical Mathematics and Scientific Computing*, organized a workshop on the modeling and numerics of electrochemical problems in the context of energy conversions (see page 101).

References

[1] P.-E. Druet, O. Klein, J. Sprekels, F. Tröltzsch, I. Yousept, *Optimal control of 3D state-constrained induction heating problems with nonlocal radiation*, SIAM J. Control Optim, **49(4)** (2011), pp. 1707–1736.

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

[3] P. Colli, G. Gilardi, P. Podio-Guidugli, J. Sprekels, *Well-posedness and long-time behavior for a nonstandard viscous Cahn–Hilliard system*, SIAM J. Appl. Math., **71** (2011), pp. 1849–1870.

[4] P. Colli, G. Gilardi, P. Podio-Guidugli, J. Sprekels, *Distributed optimal control of a nonstandard system of phase field equations*, to appear in: Contin. Mech. Thermodyn.

[5] S. Jachalski, R. Huth, G. Kitavtsev, D. Peschka, B. Wagner, *Stationary solutions for two-layer lubrication equations*, WIAS Preprint no. 1670, 2012, submitted.

[6] 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.

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

4.8 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.

Modeling, analysis, and numerics of damage processes

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 local and nonlocal Cahn–Hilliard systems is extended. In the local case, the Cahn–Hilliard system is coupled with elasticity and a unidirectional inclusion for an internal variable, describing complete or incomplete damage processes. In the nonlocal case, damage processes are incorporated in the multi-component Cahn–Hilliard system by considering the damage process as a diffusion process of voids or vacancies, being nothing but some special type of noninteracting particles of the multi-component system. For these systems, appropriate notions of weak solutions, existence results, and numerical simulations are established. For analytical and numerical investigations on the nonlocal Cahn–Hilliard system with damage, the reader is referred to the Scientific Highlights article by Jens A. Griepentrog on page 25.

***Fig. 1:** Snapshots from a numerical simulation of phase separation and damage with material-dependent elasticity tensor and time-varying loading. Damage shows alignment with phase boundaries (R"udiger Müller (LG 2))*

In the above-mentioned models, the energy is typically not simultaneously convex in all variables (i. e., displacements and damage variables). Thus, solutions of rate-independent damage and crack propagation models may be discontinuous in time. In order to derive suitable jump criteria, a vanishing viscosity analysis was carried out for damage models generalizing the results for models with a single crack. In this way, in the limit, a novel formulation is obtained for rate-independent damage models, which highlights the interplay of viscous and rate-independent effects in the jump regime and provides a better description of the energetic behavior of the system at jumps.

For a better understanding of the influence of the evolution of microdefects on the effective macroscopic behavior of materials, a two-scale damage evolution model was set up and investigated analytically. By choosing appropriate geometries and evolution laws on the microscale, this approach opens the possibility to introduce several damage variables and, thus, to model anisotropic damage phenomena.

As a further topic, the Stefan problem was investigated with a spatially inhomogeneous and anisotropic Gibbs–Thomson condition at the phase boundary. In particular, the long-time existence of weak solutions was established. A spatially inhomogeneous and anisotropic Gibbs–Thomson condition allows to model phase transitions in materials, such as the solidification of alloys, where the surface energy density depends on the position in space and on the local orientation of the interface.

Projects

The research group participates in the DFG Research Center MATHEON with the project C32 "Modeling of phase separation and damage processes in solder alloys".

Christiane Kraus participates in the interdisciplinary research group *Micro-Macro Modeling and Simulation of Liquid-Vapor Flows* of DFG and the French National Center for Scientific Research CNRS with the project "Modeling and sharp interface limits of generalized Navier–Stokes–Korteweg systems".

Further activities

The International Workshop "Modeling and Analysis of Phase Separation, Damage and Fracture" organized by Dorothee Knees (LG 2) and Christiane Kraus (LG 2), took place at WIAS from September 21 through 23 September, 2011. The lectures focused on modeling of micro and mesoscopic structure evolution (e. g. micro-cracks or micro-voids, phase separation and damage, crack propagation), analytical results for highly nonlinear elliptic and parabolic PDEs, numerical methods and on applications in physics and mechanics. Partial financial support by the MATHEON is gratefully acknowledged.

Fig. 2: *Participants of the workshop "Modeling and Analysis of Phase Separation, Damage and Fracture"*

Finally, Dorothee Knees and Christiane Kraus successfully organized a minisymposium at the 7th International Congress on Industrial and Applied Mathematics — ICIAM 2011 (Vancouver) with lectures on modeling and analysis of damage phenomena.

A Facts and Figures

(In the sequel, WIAS staff members are underlined.)

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

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

A.1.1 Calls

1. R.L. Loeffen, W2 professorship, June 28, University of Manchester, Faculty of Engineering and Physical Sciences (senior lecturer).

A.1.2 Awards and Distinctions

1. W. König, *"Idea for the Federal Republic of Learning" issued by the initiative "Germany — Land of Ideas" for the Center for Mathematics and Science Education and Hands-on Museum "INSPIRATA", chaired by W. König*, September 29, 2011.
2. A. Mielke, *Head of IMU Secretariat*.
3. ———, *Member of the Executive Committee of the International Society for Interaction of Mathematics and Mechanics (ISIMM)*.
4. ———, *Member of the IMU Berlin Einstein Foundation Program Committee*.
5. ———, *Treasurer of International Mathematical Union (IMU)*.
6. V. Spokoiny, *Mega-Grant of the Russian Government to establish a Research Group "Predictive Modeling" at the University of Physics and Technology in Moscow*.

A.1.3 Ph.D. Theses

1. I.V. Ermakov, *Applications of semiconductor lasers with optical feedback. Novel concepts for tunable lasers and chaos control*, Vrije Universiteit Brussel, Faculty of Engineering, supervisor: Dr. V. Tronciu, March 31.
2. J.E. Kim, *Microscopic description of quantum-dot vertical-cavity surface-emitting structures using Maxwell–Bloch equations*, Technische Universität Berlin, Fakultät Mathematik und Naturwissenschaften, supervisor: Priv.-Doz. Dr. U. Bandelow, May 17.
3. N. Kleemann, *Shape derivatives for diffraction by non-smooth periodic interfaces*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisors: Prof. Dr. D. Hömberg, Dr. A. Rathsfeld, August 19.
4. Ch. Mukherjee, *Large deviations for Brownian intersection measures*, Universität Leipzig, Fakultät für Mathematik und Informatik, supervisor: Prof. Dr. W. König, August 27.
5. O. Rott, *Simulation and stability of milling processes*, Technische Universität Berlin, Fakultät V — Verkehrs- und Maschinensysteme, supervisor: Prof. Dr. D. Hömberg, October 25.
6. P. Schmid, *Random processes in truncated and ordinary Weyl chambers*, Universität Leipzig, Fakultät für Mathematik und Informatik, supervisor: Prof. Dr. W. König, March 9.
7. C. Brée, *Self-compression of intense optical pulses and the filamentary regime of nonlinear optics*, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät I, supervisors: Prof. Dr. Th. Elsässer, Priv.-Doz. Dr. U. Bandelow, Prof. O. Kosareva, September 21.
8. D. Kern, *Analysis and numerics for a thermomechanical phase transition model in steel*, Technische Universität Berlin, Fakultät II – Mathematik und Naturwissenschaften, supervisor: Prof. Dr. D. Hömberg, May 26.

A.1.4 Undergraduate-degree Supervision

1. D. KUMMER, *Asymptotische Analysis für Navier-Stokes-Korteweg-Systeme mit Temperatur* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. J. Sprekels, December 7.
2. G. MORAWSKI, *Das parabolische Anderson-Modell mit allgemeinen zeitabhängigen Katalysatoren* (diploma thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, March 1.
3. J. OERTEL, *Ein funktionaler Grenzwertsatz für lange Warteschlangen* (bachelor's thesis), Technische Universität Berlin, Fakultät II — Mathematik und Naturwissenschaften, supervisor: Prof. Dr. W. König, July 1.
4. F. PLATZEK, *Zwei Verallgemeinerungen der Allen-Cahn-Gleichung für Phasentrennungsprozesse* (diploma thesis), Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, supervisor: Prof. Dr. J. Sprekels, September 20.
5. F. THEIN, *On the efficiency and condition of the core routine of the Quadrature Method of Moments (QMOM)* (diploma thesis), Otto-von-Guericke-Universität Magdeburg, Fakultät für Mathematik, supervisor: Prof. Dr. V. John, October 14.
6. U. WILBRANDT, *A posteriori Optimierung von Parametern in stabiliersierten Finite-Elemente-Methoden für Konvektions-Diffusions-Gleichungen* (master's thesis), Freie Universität Berlin, Fachbereich Mathematik und Informatik, supervisor: Prof. Dr. V. John, October 5.

A.2 Grants[1]

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

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

  "Verbundprojekt 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 sub-project "Gesamtmodell, Analysis, Gesamtsimulator" (Modeling, analysis, process simulator; in RG 4)

- **Fördermaßnahme "Wissens- und Technologietransfer — Entwicklung, Umsetzung und Professionalisierung von Verwertungskonzepten aus Mathematik, Natur- und Ingenieurwissenschaftlichen Leibniz-Einrichtungen der Sektion D und aus Helmholtz-Zentren im Nicht-Life-Science-Bereich"** (Funding program: Transfer of knowledge and technology — Development, implementation, and professionalization of transfer concepts from institutes of the Leibniz Association's Section D with a focus on mathematical, natural scientific or engineering research as well as from Helmholtz Centers not working in the life sciences)

  "Entwicklung, Umsetzung und Professionalisierung eines Verwertungskonzeptes am Weierstraß-Institut" (Development, implementation, and professionalization of the transfer strategy at the Weierstrass Institute)

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), project coordination and sub-project "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

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

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

  C9: "Simulation and optimization of semiconductor crystal growth from the melt controlled by traveling magnetic fields" (in RG 7)

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

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

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

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

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

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

C30: “Automatic reconfiguration of robotic welding cells” (in RG 4)

C32: “Modeling of phase separation and damage processes in alloys” (in LG 2)

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

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

D22: “Modeling of electronic properties of interfaces in solar cells” (in RG 1)

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

F10: “Image and signal processing in the biomedical sciences: Diffusion weighted imaging — Modeling and beyond” (in RG 6)

– **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” (until 03/11, 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)

– **Collaborative Research Center (SFB) 910**, Technische Universität Berlin, **“Kontrolle selbstorganisierender nichtlinearer Systeme: Theoretische Methoden und Anwendungskonzepte” (Control of Self-organizing Nonlinear Systems: Theoretical Methods and Concepts of Application)**

A05: “Musterbildung in mehrskaligen Systemen” (Pattern formation in systems with multiple scales; in RG 1)

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

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

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

“Simulation, Optimierung und Regelung von Gefügebildung und mechanischen Eigenschaften beim Warmwalzen von Mehrphasenstählen” (Simulation, 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)**

“Dynamics of viscous multi-layer systems with free boundaries” (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)

"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 "Micro–Macro Modelling and Simulation of Liquid–Vapor Flows"; in RG 7 and LG 2)

– **Eigene Stelle (Temporary Positions for Principal Investigators)**

"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; I. Babushkin)

– **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)

Leibniz-Gemeinschaft (Leibniz Association), Bonn and Berlin

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

"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

– A Friedrich Wilhelm Bessel awardee (in RG 1)

– 3 scholarship holders (in RG 3, RG 5, and RG 6); see page 144

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)

– ERC Advanced Grant “Analysis of multiscale systems driven by functionals” (A. Mielke in RG 1)

– EU Collaborative Project “MASH — Massive Sets of Heuristics” (participation in RG 6)

– EU Marie Curie Actions Initial Training Network PROPHET (Postgraduate Research on Photonics as an Enabling Technology), project 1.4 “Modelling of mode-locked QD lasers” (in RG 2)

Mission-oriented research (examples)

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

– 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)

– 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)

– 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. R. Henrion, Editorial Board, Nonlinear Analysis: Theory, Methods & Applications, Elsevier, Amsterdam, The Netherlands.
4. ———, Editorial Board, Set-Valued and Variational Analysis, Springer-Verlag, Dordrecht, The Netherlands.
5. ———, Editorial Board, International Journal of Management Science and Engineering Management (MSEM), World Academic Press, Liverpool, UK.
6. ———, Editorial Board, SIAM Journal on Optimization, Society for Industrial and Applied Mathematics, Philadelphia, Pennsylvania, USA.
7. ———, Editorial Board, Journal of Optimization Theory and Applications, Springer-Verlag, Dordrecht, The Netherlands.
8. D. Hömberg, Editorial Board, Applicationes Mathematicae, Institute of Mathematics of the Polish Academy of Sciences (IMPAN), Warsaw.
9. D. Knees, Editorial Board, Discrete and Continuous Dynamical Systems — Series S (DCDS-S), American Institute of Mathematical Sciences, Springfield, Missouri, USA.
10. W. König, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
11. V. Krätschmer, Editorial Board, Applied Computational Intelligence and Soft Computing, Hindawi Publishing Corporation, New York, USA.
12. P. Mathé, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.
13. ———, Editorial Board, Journal of Complexity, Elsevier, Amsterdam, The Netherlands.
14. A. Mielke, Advisory Board, Mathematische Nachrichten, WILEY-VCH Verlag, Weinheim.
15. ———, Editor-in-Chief, Journal of Nonlinear Science, Springer Science+Business Media, New York, USA.
16. ———, Editorial Board, Archive for Rational Mechanics and Analysis, Springer-Verlag, Berlin, Heidelberg.
17. ———, Editorial Board, Zeitschrift für Angewandte Mathematik und Mechanik (ZAMM), WILEY-VCH Verlag, Weinheim.
18. ———, Editorial Board, European Series in Applied and Industrial Mathematics: Control, Optimisation and Calculus of Variations, EDP Sciences, Les Ulis, France.
19. ———, Editorial Board, Mathematical Models and Methods in Applied Sciences, Imperial College Press, London, UK.
20. ———, Editor, Zeitschrift für Angewandte Mathematik und Physik (ZAMP), Birkhäuser Verlag, Basel, Switzerland.
21. H. Neidhardt, Editorial Board, Nanosystems: Physics, Chemistry, Mathematics, St. Petersburg State University of Information Technologies, Mechanics and Optics, Russia.
22. ———, Editorial Board, Advances in Mathematical Physics, Hindawi Publishing Corporation, New York, USA.
23. J. Polzehl, Editorial Board, Computational Statistics, Physica Verlag, Heidelberg.

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

24. ———, Editorial Board, Journal of Multivariate Analysis, Elsevier, Amsterdam, The Netherlands.

25. J.G.M. Schoenmakers, Editorial Board, Journal of Computational Finance, Incisive Media Investments Limited, London, UK.

26. ———, Editorial Board, Monte Carlo Methods and Applications, Walter de Gruyter, Berlin, New York, USA.

27. J. Sprekels, Editorial Board, Applications of Mathematics, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague.

28. ———, Editorial Board, Mathematics and its Applications, Annals of the Academy of Romanian Scientists, Academy of Romanian Scientists, Bucharest, Romania.

29. ———, Editor, Advances in Mathematical Sciences and Applications, Gakkōtosho, Tokyo, Japan.

30. 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 Model Order Reduction in Optimization and Control with PDEs
Berlin, January 26–28
Organized by: WIAS (RG 3)
Supported by: DFG Research Center Matheon, DFG SPP 1253

The goal of the workshop was to obtain an overview of the state of the art of the research in Germany concerning the topic of the workshop. All groups being active in this topic participated and presented their latest results. Altogether, 22 invited talks were given, and the number of participants was about 60. In a round table meeting, the possibilities of a joint proposal on the topic were discussed. However, it turned out that a few groups already launched a proposal for a DFG research unit, and it was agreed that without these groups a large proposal, like for a DFG priority programme, would be without a chance of being successful.

Mathematical Challenges of Quantum Transport in Nano-Optoelectronic Systems
Berlin, February 4–5
Organized by: WIAS (RG 1)
Supported by: DFG, WIAS

The goal of the workshop was to give mathematicians, theoretical physicists, and experimental physicists the opportunity to exchange ideas about the modeling of charge transport and of charge interaction with external fields in nano-optoelectronic devices. The models developed are important for describing the influence of light on the electrical current, for example, in solar cells and photodetectors, but also the influence of the electrical current on the light emission, for example, in light-emitting diodes. The research area is of interest for the theoretical understanding, experimental study, as well as for the efficient and optimal applicability of these systems.

The workshop with 24 participants from 8 countries featured 13 invited and five contributed talks. It was also an opportunity for young researchers to contribute to this very interesting and rapidly developing research area. Part of the contributions appeared in the journal "Nanosystems: Physics, Chemistry, Mathematics", Vol. 2, Issue 3, 2011, St. Petersburg, Russia.

Workshop on Modeling and Analysis of Phase Separation, Damage and Fracture
Berlin, September 21–23
Organized by: WIAS (LG 2), Matheon Project Group C32 "Modeling of phase separation and damage processes in alloys"
Supported by: Matheon, WIAS, Leibniz Association

Phase separation, damage, and fracture processes occur in nearly all materials and structures and can reduce the functionality and life time of materials dramatically. It is of great interest to model, analyze, and simulate these processes. In this way, it is possible to predict failure, to estimate life times, and to improve the behavior of the materials. The aim of the workshop was to bring together researchers from applied analysis, numerics, and materials sciences in order to discuss different aspects of the modeling, the mathematical properties, and the simulation of fracture, damage, and phase separation phenomena.

About 50 scientists, mainly from the Czech Republic, Italy, and Germany, participated at the workshop. In three keynote lectures and 22 other lectures, a broad range of topics from the modeling, analysis, and simulation were covered.

Asymptotic Expansions in Applied Analysis and Stochastics
Berlin, October 10–11
Organized by: WIAS (RG 6), Matheon project groups E5 "Statistical and numerical methods in modelling of financial derivatives and valuation of risk" and E10 "Image and signal processing in the biomedical sciences: Diffusion weighted imaging — Modeling and beyond"
Supported by: WIAS, DFG Research Center Matheon, European Research Council

Asymptotic expansions have been a common tool in many areas of modern applied mathematics. The workshop "Asymptotic Expansions in Applied Analysis and Stochastics" brought together experts in a variety of fields to create a fertile ground for discussion and exchange of ideas. Topics included tail expansions for diffusion processes and solutions to Fokker–Planck equations, short time expansions in PDE/Markovian and non-Markovian models, large deviations and Laplace method on Wiener space, large strike expansions in stochastic volatility models, expansions in Fourier space, asymptotic expansions in phase transitions problems.

The workshop was jointly organized by the WIAS research groups *Thermodynamic Modeling and Analysis of Phase Transitions* and *Stochastic Algorithms and Nonparametric Statistics* (scientific board: W. Dreyer, P.K. Friz, J. Schoenmakers).

The two-day workshop attracted around 30 participants and featured 7 invited speakers, two of them senior researchers from the U.S. The meeting served in particular as a platform to exchange new approaches for similar mathematical questions in applications seemingly as far apart as volatility smile modeling and phase transitions in many-particle systems.

Dynamics of Oscillator Populations
Berlin, October 31
Organized by: WIAS (RG 2), Humboldt-Universität zu Berlin, Universität Potsdam

This workshop, attended by 30 participants from three countries, was based on a long-lasting successful collaboration between scientists from WIAS, Humboldt-Universität zu Berlin, Universität Potsdam, Istituto dei Sistemi Complessi (Florence, Italy), and the Ukrainian Academy of Sciences (Kiev). The topic of coupled oscillator populations is a recently very active field of research with various applications, e.g., in neuroscience, communication technology, or theoretical biology. Ten talks were given.

Mathematical Modeling and Experimental Investigation of Electrochemical Processes in Energy Storage Systems (MODELCHEM 2011)
Berlin, November 21–22
Organized by: WIAS (RG 3 and RG 7)

Electrochemical storage systems like batteries and fuel cells play a crucial role in the development of future energy supply systems. For several years, WIAS researchers have been active in the development of detailed macroscopic simulation models for several aspects of electrochemical devices. The workshop intended to share this experience with partners from research in applied mathematics and electrochemistry, to intensify existing collaborations, and to identify directions for further research in the field. Fourteen invited speakers from Germany and Austria agreed to present their research at this event. Overall, the workshop had 36 participants.

Berlin Workshop on Statistics and Neuroimaging 2011
Berlin, November 23–25
Organized by: WIAS (RG 6), Matheon Project Group F10 "Image and signal processing in the biomedical sciences: Diffusion weighted imaging — Modeling and beyond"
Supported by: WIAS, Bernstein Center for Computational Neuroscience Berlin, and DFG Research Center Matheon

The neurosciences have seen a dramatic development in recent years and draw their challenges and interest from the combination of different disciplines like mathematics, physics, medicine, psychology, neurology, and computer sciences. The workshop "Statistics and Neuroimaging 2011" held at WIAS brought together internationally recognized experts in the field to create a fertile ground for discussion and exchange.

The topics covered by the 16 invited and 5 contributed talks included MR physics and data acquisition, statistical modeling of diffusion-weighted data, clinical applications of diffusion-weighted MRI, statistical modeling of functional MRI data and software development for MRI.

The workshop had 61 participants from 8 countries worldwide.

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

25TH IFIP TC 7 CONFERENCE ON SYSTEM MODELING AND OPTIMIZATION
Berlin, September 12–16
Organized by: WIAS (RG 4), Technische Universität (TU) Berlin
Supported by: DFG Research Center MATHEON, DFG, WIAS, TU Berlin, European Science Foundation, INRIA, European Patent Office

The conference was co-organized by D. Hömberg (RG 4) and F. Tröltzsch (TU Berlin). It is part of a biennial conference series with preceding conferences in Buenos Aires (2009), Cracow (2007), and Turin (2005). With 315 participants from 37 countries, 288 lectures, the majority of them delivered in 67 minisymposia and 8 contributed sessions, the conference became a great success. It showed the attractiveness of the IFIP TC 7 concept linking research in abstract mathematical optimization and control theory and building a bridge to numerical methods and applications in various fields.

A.4.3 Oberwolfach Workshops co-organized by WIAS

VARIATIONAL METHODS FOR EVOLUTION
Oberwolfach, December 4–10
Organized by: Alexander Mielke (RG 1), Felix Otto (Leipzig), Giuseppe Savaré (Pavia), Ulisse Stefanelli (Pavia)

About 50 mathematicians and applied scientists discussed a wide range of topics, including large deviation and variational principles, rate-independent evolutions and gradient flows, heat flows in metric-measure spaces, applications of optimal transport and entropy-entropy dissipation methods and many more. During the workshop, the Oberwolfach Prize 2010 for excellent achievements in analysis and applied mathematics was jointly awarded to Nicola Gigli (Nice) and László Székelyhidi (Bonn).

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

1. P. Friz, chair of the invited session “Rough Path Analysis”, *35th Conference on Stochastic Processes and their Applications*, Universidad Nacional Autónoma de México of Oaxaca, Instituto de Matemáticas, June 19–25.
2. ———, co-organizer, *Workshop Rough Paths and Numerical Integration Methods*, Philipps-Universität Marburg, Fachbereich Mathematik und Informatik, September 21–23.
3. U. Bandelow, member of the Organizing Committee, *11th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD 2011)*, Rome, Italy, September 5 – October 8.
4. W. Dreyer, co-organizer of a mathematics-for-industry meeting on incompressible two-phase flow, *Multiscale Coupling of Complex Models (CEMRACS ’11)*, Centre International de Rencontres Mathématiques, Marseille, France, August 16–18.
5. R. Henrion, co-organizer of the minisymposium “MS12 Advances in Probabilistic Programming I-II”, *25th IFIP TC 7 Conference on System Modeling and Optimization*, Technische Universität Berlin, September 12–16.
6. D. Hömberg, co-organizer, *25th IFIP TC 7 Conference on System Modeling and Optimization*, Technische Universität Berlin, September 12–16.
7. ———, member of the Scientific Committee, *3rd International Conference on Distortion Engineering 2011*, Bremen, September 14–16.
8. V. John, member of the Local Advisory Committee and co-organizer of the minisymposium “Finite Element Methods for Convection-Dominated Problems”, *16th International Conference on Finite Elements in Flow Problems*, Munich, March 23–25.
9. D. Knees, co-organizer of the minisymposium “Modeling and Analysis of Phase Separation, Damage and Fracture”, *7th International Congress on Industrial and Applied Mathematics (ICIAM 2011)*, Society for Industrial and Applied Mathematics, Vancouver, Canada, July 18–22.
10. W. König, organizer, *Berlin-Leipzig Seminar on Analysis and Probability Theory*, Technische Universität Dortmund, Fakultät für Mathematik, January 14.
11. ———, organizer, *Berlin-Leipzig Seminar on Analysis and Probability Theory*, Technische Universität Clausthal, Institut für Mathematik, July 8.
12. ———, member of the Local Organizing Committee and coordinator, *Summer School of the Berlin Mathematical School 2011 “Random Motions and Random Graphs”*, Technische Universität Berlin, Institut für Mathematik, September 27 – October 7.
13. ———, organizer, *Berlin-Leipzig Seminar on Analysis and Probability Theory*, Technische Universität Braunschweig, Institut für Analysis und Algebra, November 4.
14. Ch. Kraus, co-organizer of the minisymposium “Modeling and Analysis of Phase Separation, Damage and Fracture”, *7th International Congress on Industrial and Applied Mathematics (ICIAM 2011)*, Society for Industrial and Applied Mathematics, Vancouver, Canada, July 18–22.
15. ———, co-organizer of a mathematics-for-industry meeting on incompressible two-phase flow, *Multiscale Coupling of Complex Models (CEMRACS ’11)*, Centre International de Recontres Mathématiques, Marseille, France, August 16–18.

[3] Membership 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 WIAS staff members.

16. K. Krumbiegel, co-organizer of the minisymposium “Practical Applications of Optimization with PDE Constraints”, *7th International Congress on Industrial and Applied Mathematics (ICIAM 2011)*, Society for Industrial and Applied Mathematics, Vancouver, Canada, July 18–22.
17. ———, co-organizer of the minisymposium “MS16 Modeling and Inverse Problems in Scatterometry”, *25th IFIP TC 7 Conference on System Modeling and Optimization*, Technische Universität Berlin, September 12–16.
18. Ch. Landry, co-organizer of the minisymposium “MS15 Optimal Control in Robotics I-II”, *25th IFIP TC 7 Conference on System Modeling and Optimization*, Technische Universität Berlin, September 12–16.
19. A. Mielke, co-organizer, *Autumn School “Mathematical Principles for and Advances in Continuum Mechanics”*, Centro di Ricerca Matematica “Ennio De Giorgi”, Pisa, Italy, November 7–12.
20. ———, co-organizer, *Workshop “Variational Methods for Evolution”*, Mathematisches Forschungsinstitut Oberwolfach, December 4–10.
21. A. Petrov, co-organizer of the minisymposium “Vibrations with Unilateral Constraints”, *7th International Congress on Industrial and Applied Mathematics*, Society for Industrial and Applied Mathematics, Vancouver, Canada, July 18–22.
22. A. Rathsfeld, co-organizer of the minisymposium “MS16 Modeling and Inverse Problems in Scatterometry”, *25th IFIP TC 7 Conference on System Modeling and Optimization*, Technische Universität Berlin, September 12–16.
23. V. Spokoiny, co-organizer, *International Workshop “Structural Methods of Data Analysis and Optimization”*, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, Russia, December 15–17.
24. V. Tronciu, member of the Advisory Board, *NANO-2011 Cooperation and Networking of Universities and Research Institutes — Study by Doing Research*, Academy of Science, Institute of Electronic Engineering and Nanotechnologies, Kishinev, Moldova, October 6–9.
25. A.G. Vladimirov, co-organizer of the session “Instabilities and Solitons in Nonlinear Photonics: Part 2”, *Progress in Electromagnetics Research Symposium*, Marrakesh, Morocco, March 20–23.
26. ———, member of the Program Commitee EH, *Conference on Lasers and Electro-Optics — European Quantum Electronics Conference (CLEO®/Europe — EQEC 2011)*, Munich, May 22–26.
27. ———, member of the Organizing Commitee, *International Workshop “Nonlinear Photonics: Theory, Materials, Applications”*, St. Petersburg State University and the State University of Information Technologies, Mechanics and Optics, Russia, August 24–26.
28. B. Wagner, organizer, *Mathematical Modelling of Organic Solar Cells*, Technische Universität Berlin, September 26–27.
29. W. Wagner, member of the Scientific Committee, *8th International Conference on Large-Scale Scientific Computations*, Institute of Information and Communication Technologies, Bulgarian Academy of Sciences and Society for Industrial and Applied Mathematics (SIAM), Sozopol, Bulgaria, June 6–10.

A.6 Publications

A.6.1 Monographs

[1] K. Tabelow, B. Whitcher, eds., *Magnetic Resonance Imaging in R*, vol. 44 of Journal of Statistical Software, American Statistical Association, 2011, 320 pages.

A.6.2 Editorship of Proceedings and Collected Editions

Proceedings and Collected Editions (to appear)

[1] J.-D. Deuschel, B. Gentz, W. König, M. von Renesse, M. Scheutzow, U. Schmock, eds., *Probability in Complex Physical Systems, in Honour of Erwin Bolthausen and Jürgen Gärtner*, vol. 11 of Springer Proceedings in Mathematics, Springer, Berlin Heidelberg.

A.6.3 Outstanding Contributions to Monographs

[1] O. Schenk, K. Gärtner, *PARDISO, in: Encyclopedia of Parallel Computing, Part 16*, D. Padua, ed., Springer, New York et al., 2011, pp. 1458–1464.

[2] A. Mielke, *Chapter: Differential, Energetic, and Metric Formulations for Rate-Independent Processes, in: Nonlinear PDE's and Applications, C.I.M.E. Summer School, Cetraro, Italy 2008*, L. Ambrosio, G. Savaré, eds., vol. 2028 of Lecture Notes in Mathematics, Springer, Berlin Heidelberg, 2011, pp. 87–167.

Contributions to Monographs (to appear)

[1] K. Gärtner, H. Si, A. Rand, N. Walkington, *Chapter 19: 3D Delaunay Mesh Generation, in: Combinatorial Scientific Computing*, U. Naumann, O. Schenk, eds., CRC Computational Science, Chapman & Hall.

[2] J. Polzehl, K. Tabelow, *Chapter 4: Structural Adaptive Smoothing: Principles and Applications in Imaging, in: Mathematical Methods for Signal and Image Analysis and Representation*, L. Florack, R. Duits, G. Jongbloed, M.-C. van Lieshout, L. Davies, eds., vol. 41 of Computational Imaging and Vision, Springer, London et al.

A.6.4 Articles in Refereed Journals[4]

[1] I. Babushkin, St. Skupin, A. Husakou, Ch. Köhler, E. Cabrera-Granado, L. Bergé, J. Herrmann, *Tailoring terahertz radiation by controlling tunnel photoionization events in gases*, New J. Phys., 13 (2011), pp. 123029/1–123029/16.

[2] M. Beiglboeck, P. Friz, St. Sturm, *Is the minimum value of an option on variance generated by local volatility?*, SIAM J. Financial Math., 2 (2011), pp. 213–220.

[3] M. Caruana, P. Friz, H. Oberhauser, *A (rough) pathwise approach to a class of nonlinear SPDEs*, Ann. Inst. H. Poincare Anal. Non Lineaire, 28 (2011), pp. 27–46.

[4] Th. Cass, P. Friz, *Malliavin calculus and rough paths*, Bull. Sci. Math., 135 (2011), pp. 542–556.

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[5] P. Friz, S. Gerhold, A. Gulisashvili, S. Sturm, *On refined volatility smile expansion in the Heston model*, Quant. Finance, 11 (2011), pp. 1151–1164.

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[7] P. Friz, N. Victoir, *A note on higher dimensional p-variation*, Electron. J. Probab., 16 (2011), pp. 1880–1899.

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[9] H. Oberhauser, P. Friz, *On the splitting-up method for rough (partial) differential equations*, J. Differential Equations, 251 (2011), pp. 316–338.

[10] G. Aki, J. Dolbeult, Ch. Sparber, *Thermal effects in gravitational Hartree systems*, Ann. Henri Poincare, 26 (2011), pp. 1055–1079.

[11] S. Amiranashvili, A. Demircan, *Ultrashort optical pulse propagation in terms of analytic signal*, Adv. Opt. Technol., (2011), pp. 989515/1–989515/8.

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[12] C. Brée, A. Demircan, J. Bethge, E.T.J. Nibbering, St. Skupin, L. Bergé, G. Steinmeyer, *Filamentary pulse self-compression: The impact of the cell windows*, Preprint no. 1606, WIAS, Berlin, 2011.

[13] C. Brée, A. Demircan, G. Steinmeyer, *Kramers–Kronig relations and high order nonlinear susceptibilities*, Preprint no. 1651, WIAS, Berlin, 2011.

[14] M. Augustin, A. Caiazzo, A. Fiebach, J. Fuhrmann, V. John, A. Linke, R. Umla, *An assessment of discretizations for convection-dominated convection-diffusion equations*, Preprint no. 1609, WIAS, Berlin, 2011.

[15] W. Dreyer, M. Hantke, G. Warnecke, *Exact solutions to the Riemann problem for compressible isothermal Euler equations for two phase flows with and without phase transition*, Preprint no. 1620, WIAS, Berlin, 2011.

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

[17] J. Elschner, G. Hu, *An optimization method in inverse elastic scattering for one-dimensional grating profiles*, Preprint no. 1622, WIAS, Berlin, 2011.

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

[18] ———, *Uniqueness in inverse scattering of elastic waves by three-dimensional polyhedral diffraction gratings*, Preprint no. 1591, WIAS, Berlin, 2011.

[19] A. Bradji, J. Fuhrmann, *Some abstract error estimates of a finite volume scheme for a nonstationary heat equation on general nonconforming multidimensional spatial meshes*, Preprint no. 1660, WIAS, Berlin, 2011.

[20] R. Eymard, J. Fuhrmann, A. Linke, *MAC schemes on triangular Delaunay meshes*, Preprint no. 1654, WIAS, Berlin, 2011.

[21] A. Glitzky, *An electronic model for solar cells including active interfaces and energy resolved defect densities*, Preprint no. 1663, WIAS, Berlin, 2011.

[22] A. Glitzky, A. Mielke, *A gradient structure for systems coupling reaction-diffusion effects in bulk and interfaces*, Preprint no. 1603, WIAS, Berlin, 2011.

[23] F. Castell, O. Gün, G. Maillard, *Parabolic Anderson model with finite number of moving catalysts*, Preprint no. 1669, WIAS, Berlin, 2011.

[24] S. Heinz, *Quasiconvexity equals rank-one convexity for isotropic sets of 2x2 matrices*, Preprint no. 1637, WIAS, Berlin, 2011.

[25] K. Hackl, S. Heinz, A. Mielke, *A model for the evolution of laminates in finite-strain elastoplasticity*, Preprint no. 1655, WIAS, Berlin, 2011.

[26] G. Colombo, R. Henrion, N.D. Hoang, B.S. Mordukhovich, *Optimal control of the sweeping process*, Preprint no. 1619, WIAS, Berlin, 2011.

[27] R. Henrion, A. Seeger, *Condition number and eccentricity of a closed convex cone*, Preprint no. 1594, WIAS, Berlin, 2011.

[28] M. Gerdts, R. Henrion, D. Hömberg, Ch. Landry, *Path planning and collision avoidance for robots*, Preprint no. 1658, WIAS, Berlin, 2011.

[29] D. Hömberg, K. Krumbiegel, J. Rehberg, *Boundary coefficient control — A maximal parabolic regularity approach*, Preprint no. 1599, WIAS, Berlin, 2011.

[30] D. Hömberg, E. Uhlmann, O. Rott, P. Rasper, *Development of a stability prediction tool for the identification of stable milling processes*, Preprint no. 1588, WIAS, Berlin, 2011.

[31] D. Hömberg, J. Liu, N. Togobytska, *Identification of the thermal growth characteristics of coagulated tumor tissue in laser-induced thermotherapy*, Preprint no. 1600, WIAS, Berlin, 2011.

[32] G. Hu, *Inverse wave scattering by unbounded obstacles: Uniqueness for the two-dimensional Helmholtz equation*, Preprint no. 1592, WIAS, Berlin, 2011.

[33] S. Jachalski, R. Huth, G. Kitavtsev, D. Peschka, B. Wagner, *Stationary solutions for two-layer lubrication equations*, Preprint no. 1670, WIAS, Berlin, 2011.

[34] S. Jansen, *Fermionic and bosonic Laughlin state on thick cylinders*, Preprint no. 1642, WIAS, Berlin, 2011.

[35] ———, *Mayer and virial series at low temperature*, Preprint no. 1649, WIAS, Berlin, 2011.

[36] S. Jansen, W. König, B. Metzger, *Large deviations for cluster size distributions in a continuous classical many-body system*, Preprint no. 1632, WIAS, Berlin, 2011.

[37] V. John, J. Novo, *On (essentially) non-oscillatory discretizations of evolutionary convection-diffusion equations*, Preprint no. 1656, WIAS, Berlin, 2011.

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

[39] W. Hackbusch, V. John, A. Khachatryan, C. Suciu, *A numerical method for the simulation of an aggregation-driven population balance system*, Preprint no. 1621, WIAS, Berlin, 2011.

[40] D. Knees, R. Rossi, Ch. Zanini, *A vanishing viscosity approach to a rate-independent damage model*, Preprint no. 1633, WIAS, Berlin, 2011.

[41] D. Knees, A. Schröder, *Computational aspects of quasi-static crack propagation*, Preprint no. 1611, WIAS, Berlin, 2011.

[42] A. Fiaschi, D. Knees, S. Reichelt, *Global higher integrability of minimizers of variational problems with mixed boundary conditions*, Preprint no. 1664, WIAS, Berlin, 2011.

[43] W. König, Ch. Mukherjee, *Large deviations for Brownian intersection measures*, Preprint no. 1610, WIAS, Berlin, 2011.

[44] J. Köcher, W. König, *The longest excursion of a random interacting polymer*, Preprint no. 1596, WIAS, Berlin, 2011.

[45] W. König, M. Salvi, T. Wolff, *Large deviations for the local times of a random walk among random conductances*, Preprint no. 1605, WIAS, Berlin, 2011.

[46] M. Liero, Th. Roche, *Rigorous derivation of a plate theory in linear elastoplasticity via Gamma convergence*, Preprint no. 1636, WIAS, Berlin, 2011.

[47] M. Liero, U. Stefanelli, *The elliptic-regularization principle in Lagrangian mechanics*, Preprint no. 1662, WIAS, Berlin, 2011.

[48] K. Galvin, A. Linke, L. Rebholz, N. Wilson, *Stabilizing poor mass conservation in incompressible flow problems with large irrotational forcing and application to thermal convection*, Preprint no. 1671, WIAS, Berlin, 2011.

[49] A. Linke, L.G. Rebholz, N.E. Wilson, *On the convergence rate of grad-div stabilized Taylor–Hood to Scott–Vogelius solutions for incompressible flow problems*, Preprint no. 1589, WIAS, Berlin, 2011.

[50] B. Metzger, *An effective medium approach to the asymptotics of the statistical moments of the parabolic Anderson model and Lifshitz tails*, Preprint no. 1623, WIAS, Berlin, 2011.

[51] A. Mielke, *Emergence of rate-independent dissipation from viscous systems with wiggly energies*, Preprint no. 1643, WIAS, Berlin, 2011.

[52] ———, *Generalized Prandtl–Ishlinskii operators arising from homogenization and dimension reduction*, Preprint no. 1612, WIAS, Berlin, 2011.

[53] ———, *Geodesic convexity of the relative entropy in reversible Markov chains*, Preprint no. 1650, WIAS, Berlin, 2011.

[54] ———, *Thermomechanical modeling of energy-reaction-diffusion systems, including bulk-interface interactions*, Preprint no. 1661, WIAS, Berlin, 2011.

[55] St. Arnrich, A. Mielke, M.A. Peletier, G. Savaré, M. Veneroni, *Passing to the limit in a Wasserstein gradient flow: From diffusion to reaction*, Preprint no. 1593, WIAS, Berlin, 2011.

[56] A. Mielke, R. Rossi, G. Savaré, *Nonsmooth analysis of doubly nonlinear evolution equations*, Preprint no. 1613, WIAS, Berlin, 2011.

[57] A. Mielke, U. Stefanelli, *Linearized plasticity is the evolutionary Gamma limit of finite plasticity*, Preprint no. 1617, WIAS, Berlin, 2011.

[58] M. Malamud, H. Neidhardt, *Sturm–Liouville boundary value problems with operator potentials and unitary equivalence*, Preprint no. 1595, WIAS, Berlin, 2011.

[59] O. Omel'chenko, L. Recke, *Existence, local uniqueness and asymptotic approximation of spike solutions to singularly perturbed elliptic problems*, Preprint no. 1607, WIAS, Berlin, 2011.

[60] D. Belomestny, V. Panov, *Abelian theorems for stochastic volatility models with application to the estimation of jump activity of volatility*, Preprint no. 1631, WIAS, Berlin, 2011.

[61] R.I.A. Patterson, W. Wagner, *A stochastic weighted particle method for coagulation-advection problems*, Preprint no. 1641, WIAS, Berlin, 2011.

[62] R.I.A. Patterson, M. Kraft, W. Wagner, *Stochastic weighted particle methods for population balance equations*, Preprint no. 1597, WIAS, Berlin, 2011.

[63] L. Paoli, A. Petrov, *Existence result for a class of generalized standard materials with thermomechanical coupling*, Preprint no. 1635, WIAS, Berlin, 2011.

[64] ———, *Global existence result for phase transformations with heat transfer in shape memory alloys*, Preprint no. 1608, WIAS, Berlin, 2011.

[65] ———, *Global existence result for thermoviscoelastic problems with hysteresis*, Preprint no. 1616, WIAS, Berlin, 2011.

[66] ———, *Thermodynamics of multiphase problems in viscoelasticity*, Preprint no. 1628, WIAS, Berlin, 2011.

[67] M. Radziunas, K. Staliunas, *Spatial rocking phenomenon in broad area semiconductor lasers*, Preprint no. 1598, WIAS, Berlin, 2011.

[68] A. Rathsfeld, *Shape derivatives for the scattering by biperiodic gratings*, Preprint no. 1640, WIAS, Berlin, 2011.

[69] A. ter Elst, J. Rehberg, *L^∞-estimates for divergence operators on bad domains*, Preprint no. 1587, WIAS, Berlin, 2011.

[70] R. Schlundt, F.-J. Schmückle, W. Heinrich, *Shifted linear systems in electromagnetics. Part II: Systems with multiple right-hand sides*, Preprint no. 1646, WIAS, Berlin, 2011.

[71] G. Schmidt, *Conical diffraction by multilayer gratings: A recursive integral equations approach*, Preprint no. 1601, WIAS, Berlin, 2011.

[72] A. Papapantoleon, J.G.M. Schoenmakers, D. Skovmand, *Efficient and accurate log-Lévy approximations to Lévy driven LIBOR models*, Preprint no. 1614, WIAS, Berlin, 2011.

[73] S. Balder, A. Mahayni, J.G.M. Schoenmakers, *Primal-dual linear Monte Carlo algorithm for multiple stopping — An application to flexible caps*, Preprint no. 1666, WIAS, Berlin, 2011.

[74] D. Belomestny, J.G.M. Schoenmakers, *Multilevel dual approach for pricing American style derivatives*, Preprint no. 1647, WIAS, Berlin, 2011.

[75] Ch. Bender, J.G.M. Schoenmakers, J. Zhang, *Dual representations for general multiple stopping problems*, Preprint no. 1665, WIAS, Berlin, 2011.

[76] G.N. Milstein, V. Spokoiny, *Martingale approach in pricing European options under regime-switching*, Preprint no. 1645, WIAS, Berlin, 2011.

[77] P. Colli, G. Gilardi, P. Podio-Guidugli, J. Sprekels, *An asymptotic analysis for a nonstandard Cahn–Hilliard system with viscosity*, Preprint no. 1652, WIAS, Berlin, 2011.

[78] ———, *Distributed optimal control of a nonstandard system of phase field equations*, Preprint no. 1630, WIAS, Berlin, 2011.

[79] ———, *Well-posedness and long-time behavior for a nonstandard viscous Cahn–Hilliard system*, Preprint no. 1602, WIAS, Berlin, 2011.

[80] H. Stephan, *A mathematical framework for general classical systems and time irreversibility as its consequence*, Preprint no. 1629, WIAS, Berlin, 2011.

[81] M. Thomas, *Quasistatic damage evolution with spatial BV-regularization*, Preprint no. 1638, WIAS, Berlin, 2011.

[82] V. Tronciu, S. Schwertfeger, M. Radziunas, A. Klehr, U. Bandelow, H. Wenzel, *Amplifications of picosecond laser pulses in tapered semiconductor amplifiers: Numerical simulations versus experiments*, Preprint no. 1657, WIAS, Berlin, 2011.

[83] M. Lichtner, V. Tronciu, A.G. Vladimirov, *Improvement of output beam quality in broad area lasers with off-axis feedback*, Preprint no. 1615, WIAS, Berlin, 2011.

[84] D. Turaev, A.G. Vladimirov, S. Zelik, *Strong synchronization of weakly interacting oscillons*, Preprint no. 1659, WIAS, Berlin, 2011.

[85] J. Sieber, M. Wolfrum, M. Lichtner, S. Yanchuk, *On the stability of periodic orbits in delay equations with large delay*, Preprint no. 1586, WIAS, Berlin, 2011.

[86] M. Wolfrum, O. Omel'chenko, *Chimera states are chaotic transients*, Preprint no. 1618, WIAS, Berlin, 2011.

[87] U. Horst, Y. Hu, P. Imkeller, A. Réveillac, J. Zhang, *Forward-backward systems for expected utility maximization*, Preprint no. 1653, WIAS, Berlin, 2011.

A.7.2 Preprints/Reports in other Institutions

[1] J.D. Deuschel, P. Friz, A. Jacquier, S. Violante, *Marginal density expansions for diffusions and stochastic volatility*, arXiv:1111.2462, Cornell University Library, arXiv.org, Ithaca, USA, 2011.

[2] J. Diehl, P. Friz, H. Oberhauser, *Parabolic comparison revisited and applications*, arXiv:1102.5774, Cornell University Library, arXiv.org, Ithaca, USA, 2011.

[3] P. Friz, St. Gerhold, *Don't stay local — Extrapolation analytics for Dupire's local volatility*, arXiv:1105.1267, Cornell University Library, arXiv.org, Ithaca, USA, 2011.

[4] P. Friz, S. Riedel, *Convergence rates for the full Gaussian rough paths*, arXiv:1108.1099, Cornell University Library, arXiv.org, Ithaca, USA, 2011.

[5] ———, *Integrability of linear rough differential equations*, arXiv:1104.0577, Cornell University Library, arXiv.org, Ithaca, USA, 2011.

[6] P. Friz, N. Victoir, *A note on higher dimensional p variation*, arXiv:1102.4587, Cornell University Library, arXiv.org, Ithacs, USA, 2011.

[7] R.L. Loeffen, I. Czarna, Z. Palmowski, *Parisian ruin probability for spectrally negative Lévy processes*, arXiv:1102.4055, Cornell University Library, arXiv.org, Ithaca, USA, 2011.

[8] A.E. 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, 2011.

[9] G. Blanchard, P. Mathé, *Discrepancy principle for statistical inverse problems with application to conjugate gradient iteration*, Preprint no. 07, Universität Potsdam, Institut für Mathematik, 2011.

[10] R.I. Boţ, B. Hofmann, P. Mathé, *Regularizability of ill-posed problems and the modulus of continuity*, Preprint no. 17, Technische Universität Chemnitz, Fakultät für Mathematik, 2011.

[11] B. Hofmann, P. Mathé, *Some note on the modulus of continuity for ill-posed problems in Hilbert space*, Preprint no. 07, Technische Universität Chemnitz, Fakultät für Mathematik, 2011.

[12] J.G.M. Schoenmakers, J. Huang, *Optimal dual martingales, their analysis and application to new algorithms for Bermudan products*, Preprint no. 1825944, Social Science Research Network (SSRN) Working Paper Series, Rochester, New York, USA, 2011.

[13] W. Härdle, V. Spokoiny, *Local quantile regression*, Discussion Paper no. 2011-005, Humboldt-Universität zu Berlin, SFB 649, 2011.

[14] S. Shekar, A.J. Smith, M. Kraft, W. Wagner, *On a multivariate population balance model to describe the structure and composition of silica nanoparticles*, Technical Report no. 105, c4e-Preprint Series, Cambridge, UK, 2011.

A.8 Talks, Posters, and Contributions to Exhibitions

A.8.1 Main and Plenary Talks

1. R. Henrion, *Progress and challenges in chance-constrained programming*, SIGOPT — International Conference on Optimization 2011, June 15–17, Pfalz-Akademie Lambrecht, June 15.
2. ———, *Structure, stability and algorithmic issues of optimization problems with probabilistic constraints*, 25th IFIP TC 7 Conference on System Modeling and Optimization, September 12–16, Technische Universität Berlin, September 16.
3. D. Hömberg, *Modelling, simulation and control of multiphase steel production*, International Congress on Modelling and Simulation (MODSIM 2011), December 12–16, Perth, Australia, December 15.
4. J. Polzehl, *Statistical issues in modeling diffusion weighted magnetic resonance data*, 3rd International Conference on Statistics and Probability 2011 (IMS-China), July 8–11, Institute of Mathematical Statistics, Xian, China, July 10.
5. J. Sprekels, *Mathematical challenges in the industrial growth of semiconductor bulk single crystals*, Multiphase and Multiphysics Problems, September 25–30, Riemann International School of Mathematics, Verbania, Italy, September 26.
6. ———, *Well-posedness, asymptotic behavior and optimal control of a nonstandard phase field model for diffusive phase segregation*, Workshop on Optimal Control of Partial Differential Equations, November 28 – December 1, Wasserschloss Klaffenbach, Chemnitz, November 30.
7. W. Wagner, *Stochastic particle methods*, 8th International Conference on Large-Scale Scientific Computations, June 6–10, Institute of Information and Communication Technologies, Bulgarian Academy of Sciences and Society for Industrial and Applied Mathematics (SIAM), Sozopol, Bulgaria, June 6.

A.8.2 Scientific Talks (Invited)

1. P. Friz, *Rough path analysis and applications*, Conference in Honor of the 70th Birthday of S. R. Srinivasa Varadhan, July 11–15, National Taiwan University, Taipeh, July 14.
2. ———, *On some recent aspects of option pricing under stochastic volatility*, OMI and OCCAM Joint Workshop on Stochastic Differential Equations: Numerical Algorithms and Applications, August 8–10, University of Oxford, Oxford-Man Institute of Quantitative Finance, UK, August 8.
3. ———, *Rough analysis applied to some classes of SPDEs and related topics*, Stochastic Partial Differential Equations: Analysis, Numerics, Geometry and Modeling, September 12–17, Eidgenössische Technische Hochschule Zürich, Forschungsinstitut für Mathematik, Switzerland, September 16.
4. ———, *Gaussian rough paths*, Bonn Probability Day, Hausdorf Center for Mathematics, Universität Bonn, January 26.
5. ———, *On refined density and smile expansion in the Heston model*, Workshop “Stochastic Analysis in Finance and Insurance”, January 23–29, Mathematisches Forschungsinstitut Oberwolfach, January 29.
6. K. Götze, *Starke Lösungen für die Interaktion von starren Körpern und viskoelastischen Flüssigkeiten*, Lectures in Continuum Mechanics, Universität Kassel, Institut für Mathematik, November 7.
7. U. Stefanelli, *Evolution = Minimization?*, Friday Colloquium, Berlin Mathematical School, May 27.
8. S. Amiranashvili, *Manipulating light by light*, XXXth URSI General Assembly and Scientific Symposium of International Union of Radio Science, August 13–20, Istanbul, Turkey, August 18.

9. ———, *Can dispersive radiation feed energy into a giant wave?*, Rogue Waves, November 7–11, Dresden, November 9.

10. Th. Arnold, *On Born approximation for the scattering by rough surfaces*, 25th IFIP TC 7 Conference on System Modeling and Optimization, September 12–16, Technische Universität Berlin, September 15.

11. M. Becker, *Change point detection via universal compressors*, ECONS (Evolving Complex Networks) Spring School and Workshop, March 28–31, Potsdam Institut für Klimafolgenforschung, Wandlitz, March 29.

12. A. Caiazzo, *Implicit coupling of dissipative boundary conditions models with projection schemes for Navier–Stokes equations*, Workshop on Venous Hemodynamics, Medical Problems and Mathematical Modelling, October 25–26, Povo, Trento, Italy, October 26.

13. ———, *Model reduction approaches for simulation of cardiovascular stents and pulmonary valve*, Laboratory of Modeling and Scientific Computing, Department of Mathematics, Milan, Italy, October 27.

14. ———, *Physical- and mathematical-based reduced order modeling in computational hemodynamics*, Wroclaw University of Technology, Institute of Mathematics and Computer Science, Poland, November 16.

15. E. Diederichs, *Recent trends in large scale optimization*, ECONS (Evolving Complex Networks) Spring School and Workshop, March 28–31, Potsdam Institut für Klimafolgenforschung, Wandlitz, March 31.

16. ———, *Modellselektion durch Semidefinite Relaxation*, Jahrestagung der Deutschen Mathematiker-Vereinigung (DMV) 2011, September 19–22, Universität zu Köln, Mathematisches Institut, September 21.

17. ———, *Sparse non-Gaussian component analysis*, Structural Methods of Data Analysis and Optimization, December 15–17, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, December 16.

18. W. Dreyer, *On incompressibility*, 6th DFG-CNRS Workshop on Micro-Macro Modelling and Simulation of Liquid-Vapor Flows, January 12–14, Stuttgart, January 12.

19. ———, *Mathematical modelling of entropy induced hysteresis in many-particle systems*, Applied Math Seminar, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, March 1.

20. ———, *Mathematical models of electrodes for lithium-ion batteries*, Frühlingsschule “Evolutionsgleichungen”, April 4–6, Universität Konstanz, April 4.

21. ———, *Hysteresis and phase transition in many-particle storage systems*, INdAM Meeting “Non-linear Hyperbolic Systems of Balance Laws in Extended Thermodynamics and Kinetic Theory”, September 5–9, Cortona, Italy, September 6.

22. ———, *Modelling and simulations of the electrolyte-cathode coupling of a lithium-ion battery*, Battery Days 2011, Workshop on Modelling, Analysis and Simulation of Battery Systems, October 5–6, Universität Konstanz, October 5.

23. ———, *Thermodynamics of interfaces*, Winter School of the DFG Priority Program 1506 “Transport Processes at Fluidic Interfaces”, December 7–8, Rheinisch-Westfälische Technische Hochschule Aachen, December 7.

24. P.-E. Druet, *On existence and regularity results for the equations of magnetohydrodynamics in complex geometries*, Seminar of International Research Training Group 1529 “Mathematical Fluid Dynamics”, Technische Universität Darmstadt, June 14.

25. J. Elschner, *On scattering of time-harmonic waves by unbounded surfaces*, Workshop on Functional Analysis and Operator Theory, March 29 – April 1, Altenberg, March 29.

26. G. Faraud, *Marche aléatoires en milieu aléatoire: Le cas des arbres*, École Normale Supérieure de Lyon, Unité de Mathématiques Pures et Appliquées, Séminaire de Probabilités, France, February 3.

27. ———, *Random walks in random environment on trees*, 2011 School on Mathematical Statistical Physics, August 28 – September 9, Charles University of Prague, Center for Theoretical Study, and Academy of Sciences of the Czech Republic, Institute of Theoretical Computer Science, September 2.

28. ———, *Marche aléatoires en milieu aléatoire: Le cas des arbres*, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, November 21.

29. J. Fuhrmann, *Aspects of spatially resolved numerical modeling in electrochemical cells*, Max-Planck-Institut für komplexe dynamische Systeme, Portable Energiesysteme, Magdeburg, May 5.

30. ———, *Macroscopic models in microfluidic electrochemical devices*, Universität Ulm, Institut für Oberflächenchemie und Katalyse, May 27.

31. ———, *Finite volume schemes for nonlinear convection-diffusion problems based on the solution of local Dirichlet problems*, Conference on Simulation and Optimization, June 29 – July 1, István Széchenyi University, Györ, Hungary, June 30.

32. ———, *Electrochemical processes and porous media: Mathematical and numerical modeling*, Workshop on Simulation of Flow in Porous Media and Applications in Waste Management and CO2 Sequestration, October 3–7, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria, October 5.

33. J.A. Griepentrog, *The role of nonsmooth regularity theory in the analysis of phase separation processes*, Ehrenkolloquium anlässlich des 60. Geburtstages von PD Dr. habil. Lutz Recke, Humboldt-Universität zu Berlin, Institut für Mathematik, November 21.

34. C. Guhlke, *On the thermodynamic modelling of a lithium-ion battery*, Kraftwerk Batterie — Lösungen für Automobil und Energieversorgung, March 1–2, Aachen, March 2.

35. O. Gün, *Trap models and aging for spin glasses*, Bogazici University, Department of Mathematics, Istanbul, Turkey, December 21.

36. ———, *Parabolic Anderson model with finite number of moving catalysts*, Istanbul Center For Mathematical Sciences, Turkey, December 23.

37. ———, *Trap models and aging for spin glasses*, Koc University, Istanbul, Turkey, December 27.

38. R. Henrion, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen*, Technische Universität Ilmenau, Institut für Mathematik, April 8.

39. ———, *On calmness conditions in convex bilevel programming*, SIAM Conference on Optimization, May 16–19, Darmstadt, May 16.

40. ———, *Optimization problems with probabilistic constraints*, Sino-German Workshop on Optimization, Modeling, Methods and Applications in Industry and Management, August 15–19, Konrad-Zuse-Zentrum für Informationstechnik Berlin, August 15.

41. ———, *On joint linear probabilistic constraints with Gaussian coefficient matrix*, 25th IFIP TC 7 Conference on System Modeling and Optimization, September 12–16, Technische Universität Berlin, September 14.

42. ———, *Optimierungsaufgaben mit unsicheren Beschränkungen*, Chemnitzer Mathematisches Kolloquium, Technische Universität Chemnitz, Fakultät für Mathematik, November 17.

43. D. Hömberg, *Optimal control problems in thermomechanics*, Schwerpunktskolloquium "Analysis und Numerik", Universität Konstanz, Fachbereich Mathematik und Statistik, January 20.

44. ———, *Solid-solid phase transitions: From surface hardening of steel to laser thermo-therapy*, Southeast University, Department of Mathematics, Nanjing, Republic of China, March 28.

45. ———, *Mathematical concepts in steel manufacturing*, Fudan University, School of Mathematics, Shanghai, Republic of China, March 29.

46. ———, *Identification of phase transition kinetics from dilatometer measurements*, 19th International Conference on Computer Methods in Mechanics, May 9–12, Warsaw University of Technology, Poland, May 11.

47. ———, *Optimal boundary coefficient control for parabolic equations*, Interfaces and Discontinuities in Solids, Liquids and Crystals (INDI2011), June 20–23, Gargnano (Brescia), Italy, June 20.

48. ———, *On the phase field approach to shape and topology optimization*, Università degli Studi di Pavia, Dipartimento di Matematica "F. Casorati", Italy, November 15.

49. G. Hu, *Direct and inverse scattering of elastic waves by diffraction gratings*, Workshop 3 "Wave Propagation and Scattering, Inverse Problems and Applications in Energy and the Environment", November 21–25, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, November 24.

50. S. Jansen, *Cluster size distributions at low density and low temperature*, The University of Arizona, Department of Mathematics, Tucson, USA, April 13.

51. ———, *Fermionic and bosonic Laughlin state on thick cylinders*, Venice 2011 — Quantissima in the Serenissima, August 1–5, University of Warwick (VB), Warwick in Venice, Italy, August 4.

52. ———, *Random partitions in statistical physics*, 5th International Conference on Stochastic Analysis and its Applications, September 5–9, Hausdorff Center for Mathematics and Rheinische Friedrich-Wilhelms-Universität Bonn, September 8.

53. ———, *Statistical mechanics at low density and low temperature: Cross-over transitions from small to large cluster sizes*, 2011 School on Mathematical Statistical Physics, August 29 – September 4, Charles University of Prague, Center for Theoretical Study, and Academy of Sciences of the Czech Republic, Institute of Theoretical Computer Science, September 8.

54. ———, *Random partitions in statistical physics*, Warwick Statistical Mechanics Seminar, University of Warwick, Department of Mathematics, UK, November 17.

55. V. John, *Some topics in the discretization of scalar convection-diffusion problems*, University of Pittsburgh, Department of Mathematics, USA, May 18.

56. ———, *On the analysis and numerical analysis of some turbulence models*, Workshop "Variational Multiscale Methods (VMS 2011)", June 9–10, University of Strathclyde, Glasgow, UK, June 9.

57. ———, *Numerical methods for the simulation of population balance systems*, Particulate Flows, October 10–11, Karlsruher Institut für Technologie, Fakultät für Mathematik, October 10.

58. D. Kern, *Analysis and simulation of a thermomechanical model of phase transitions in steel*, Universität Bremen, SFB 570 "Distortion Engineering", February 2.

59. N. Kleemann, *Shape derivatives for conical diffraction by non-smooth interfaces*, Technische Universität Berlin, Institut für Mathematik, January 6.

60. ———, *Shape derivatives for conical diffraction by non-smooth interfaces*, Friedrich-Schiller-Universität Jena, Mathematisches Institut, February 11.

61. O. Klein, *Hysteresis operators for vector-valued inputs and their representation by functions on strings*, International Workshop on Hysteresis and Slow-Fast Systems (HSFS-2011), December 12–14, Lutherstadt Wittenberg, December 14.

62. D. Knees, *Numerical convergence analysis for a vanishing viscosity model in fracture mechanics*, Workshop "Perspectives in Continuum Mechanics" in Honor of Gianfranco Capriz's 85th Birthday, University of Florence, Department of Mathematics, Italy, January 28.

63. ———, *A vanishing viscosity approach in fracture mechanics*, Seminar on Partial Differential Equations, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, March 1.

64. ———, *On a vanishing viscosity approach for a model in damage mechanics*, 82th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2011), Session on Applied Analysis, April 18–21, Technische Universität Graz, Austria, April 20.

65. ———, *A survey on energy release rates*, Mini-Workshop "Mathematical Models, Analysis, and Numerical Methods for Dynamic Fracture", April 24–29, Mathematisches Forschungsinstitut Oberwolfach, April 26.

66. ———, *A vanishing viscosity approach in damage mechanics*, Interfaces and Discontinuities in Solids, Liquids and Crystals (INDI2011), June 20–24, Gargnano (Brescia), Italy, June 22.

67. ———, *A vanishing viscosity approach in damage mechanics*, Workshop "Variational Methods for Evolution", December 5–10, Mathematisches Forschungsinstitut Oberwolfach, December 5.

68. ———, *Analysis und Numerik für quasistatische Rissausbreitung*, Lectures in Continuum Mechanics, Universität Kassel, Fachbereich für Mathematik und Naturwissenschaften, December 12.

69. W. König, *Phase transitions for a dilute particle system with Lennard–Jones potential*, Ludwig-Maximilians-Universität München, Mathematisches Institut, January 20.

70. ———, *Upper tails of self-intersection local times: Survey of proof techniques*, University of Warwick, Mathematics Institute, Coventry, UK, February 17.

71. ———, *Ordered random walks*, University of California at Los Angeles, Department of Mathematics, USA, April 4.

72. ———, *A variational formula for the free energy of a many-Boson system*, University of California at Los Angeles, Department of Mathematics, USA, April 11.

73. ———, *The universality classes in the parabolic Anderson model*, Technische Universität Dresden, Institut für Analysis, June 24.

74. ———, *Eigenvalue order statistics for the heat equation with random potential*, Extreme Value Statistics in Mathematics, Physics and Beyond, July 4–8, Lorentz Center, International Center for Workshops in the Sciences, Leiden, The Netherlands, July 6.

75. ———, *Eigenvalue order statistics and mass concentration in the parabolic Anderson model*, Berlin-Leipzig Seminar on Analysis and Probability Theory, Technische Universität Clausthal, Institut für Mathematik, July 8.

76. ———, *The parabolic Anderson model*, 5 talks, 2011 School on Mathematical Statistical Physics, September 4–9, Charles University of Prague, Center for Theoretical Study, and Academy of Sciences of the Czech Republic, Institute of Theoretical Computer Science, September 5–9.

77. ———, *Localisation of the parabolic Anderson model in one island*, Jahrestagung der Deutschen Mathematiker-Vereinigung (DMV) 2011, September 20–22, Universität zu Köln, Mathematisches Institut, September 20.

78. ———, *Large deviations for cluster size distributions in a classical many-body system*, Università Ca' Foscari Venezia, Dipartimento di Management, Italy, October 13.

79. ———, *Large deviations for cluster size distributions in a classical many-body system*, 10th Workshop "Stochastic Analysis on Large Scale Interacting Systems", December 5–7, Kochi University, Faculty of Science, Shikoku, Japan, December 6.

80. ———, *Eigenvalue order statistics and mass concentration in the parabolic Anderson model*, Tokyo Institute of Technology, Department of Mathematics, Japan, December 9.

81. ———, *Eigenvalue order statistics and mass concentration in the parabolic Anderson model*, Technische Universität München, Fakultät für Mathematik, December 21.

82. ———, *Large deviations for cluster size distributions in a classical many-body system*, Universität Augsburg, Institut für Mathematik, December 22.

83. TH. KOPRUCKI, *Semi-classical modeling of quantum dot lasers with microscopic treatment of Coulomb scattering*, Universität Bremen, Institut für Theoretische Physik, February 23.

84. CH. KRAUS, *Diffuse interface systems for phase separation and damage*, Seminar on Partial Differential Equations, Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague, May 3.

85. K. KRUMBIEGEL, *Optimal control approach for production of modern multiphase steels*, International Congress on Industrial and Applied Mathematics (ICIAM), July 18–22, Vancouver, Canada, July 18.

86. ———, *Superconvergence properties for semilinear elliptic boundary control problems*, 25th IFIP TC 7 Conference on System Modeling and Optimization, September 12–16, Technische Universität Berlin, September 15.

87. CH. LANDRY, *Time-optimal control for robot motion planning*, Universität Bayreuth, Lehrstuhl für Ingenieurmathematik, June 6.

88. ———, *Path-planning with collision avoidance in automotive industry*, 25th IFIP TC 7 Conference on System Modeling and Optimization, September 12–16, Technische Universität Berlin, September 16.

89. A. LINKE, *MAC schemes on triangular Delaunay meshes*, Conference on Simulation and Optimization, June 29 – July 1, István Széchenyi University, Györ, Hungary, June 29.

90. A. LINKE, *Weak mass conservation in discretizations for the incompressible Navier–Stokes equations*, Clemson University, Department of Mathematical Sciences, USA, July 27.

91. ———, *Weak mass conservation in discretizations for the incompressible Navier–Stokes equations*, University of Manchester, School of Mathematics, UK, September 29.

92. R.L. LOEFFEN, *Option pricing in affine term structure models via spectral representations*, Seminar in Mathematical Finance, Universität Wien, Fakultät für Mathematik, Austria, January 31.

93. ———, *Two methods for pricing European options*, Colloquia on Probability and Statistics 2011, University of Bern, Institute of Mathematical Statistics and Actuarial Science, Switzerland, May 5.

94. ———, *Some discrete-time stochastic optimal control problems in finance*, 12 talks, University of Wroclaw, Faculty of Mathematics and Computer Science, Poland, May 12 – June 3.

95. ———, *Applying spectral representations for CBI processes to finance*, Stochastic Networks and Related Topics III, May 22–25, Mathematical Research and Conference Center in Bedlewo, Poland, May 24.

96. P. MATHÉ, *Conjugate gradient iteration with noisy data*, Foundations of Computational Mathematics (FoCM'11), July 4–14, Budapest, Hungary, July 6.

97. ———, *Conjugate gradient iteration under white noise*, International Conference on Scientific Computing (SC2011), October 10–14, Università di Cagliari, Dipartimento di Matematica e Informatica, Cagliari, Italy, October 14.

98. A. MIELKE, *Evolution for dissipative materials at finite strains*, From Polymer Physics to Rubber Elasticity, January 17–19, Institut National de Recherche en Informatique et en Automatique (INRIA), Paris, France, January 19.

99. ———, *Complex hysteresis operators arising from homogenization and dimension reduction*, 8th International Symposium on Hysteresis Modelling and Micromagnetics (HMM2011), Session "Mathematics of Hysteresis II", May 9–11, Università degli Studi di Trento, Centro Internazionale per la Ricerca Matematica, Levico Terme, Italy, May 10.

100. ———, *Thermodynamical modeling of bulk-interface interaction in reaction-diffusion systems*, Interfaces and Discontinuities in Solids, Liquids and Crystals (INDI2011), June 20–23, Gargnano (Brescia), Italy, June 20.

101. ———, *Remarks on evolutionary multiscale systems driven by functionals*, Intellectual Challenges in Multiscale Modeling of Solids, July 4–5, Oxford University, Mathematical Institute, UK, July 4.

102. ———, *Geometry and thermodynamics for the coupling of quantum mechanics and dissipative systems*, Workshop “Applied Dynamics and Geometric Mechanics”, August 15–19, Mathematisches Forschungsinstitut Oberwolfach, August 16.

103. ———, *Multiscale problems in systems driven by functionals*, 3 talks, ISAM-TopMath Summer School 2011 on Variational Methods, September 12–16, Technische Universität München, Fakultät für Mathematik, September 12–13.

104. ———, *Mathematical approaches to thermodynamic modeling*, 4 talks, Autumn School on Mathematical Principles for and Advances in Continuum Mechanics, November 7–12, Centro di Ricerca Matematica “Ennio De Giorgi”, Pisa, Italy, November 8–11.

105. A. Möller, *Capacity planning in energy networks by probabilistic programming*, 25th IFIP TC 7 Conference on System Modeling and Optimization, September 12–16, Technische Universität Berlin, September 14.

106. H.-J. Mucha, *Method selection in cluster analysis followed by built-in validation*, Second Bilateral German-Polish Symposium on Data Analysis and Its Applications (GPSDAA 2011), April 14–16, Cracow University of Economics, Poland, April 16.

107. R. Müller, *Combined model for phase separation and damage*, Seminar of the Collaborative Research Center (SFB) 611, Universität Bonn, Abteilung Mathematische Methoden der Physik, November 22.

108. H. Neidhardt, *Comments on the Landauer–Büttiker formula and its applications*, Quantum Transport Days, November 14–15, Université Aix-Marseille 2, Centre de Physique Théorique, France, November 14.

109. R.I.A. Patterson, *Simulating coagulating particles with advection*, University of Cambridge, Department of Chemical Engineering, UK, May 3.

110. ———, *Simulating coagulating particles in flows*, University of Cambridge, Department of Chemical Engineering, UK, October 17.

111. D. Peschka, *Liquid/liquid dewetting-stationary solutions*, Max-Planck-Institut für Mathematik in den Naturwissenschaften, AG Musterbildung, Energielandschaften und Skalierungsgesetze, Leipzig, October 5.

112. ———, *Stationary solutions in liquid/liquid dewetting*, University of California at Los Angeles, Department of Mathematics, USA, November 9.

113. A. Petrov, *Sur la modélisation mathématique de matériaux à mémoire de forme*, Université de Lyon, Institut Camille Jordan, France, May 13.

114. M. Radziunas, *Broadening of mode-locking pulses in quantum-dot semiconductor lasers: Simulation, analysis and experiments*, International Workshop “Nonlinear Photonis: Theory, Materials, Applications”, August 24–26, St. Petersburg, Russia, August 24.

115. A. Rathsfeld, *On Born approximation for the scattering by rough surfaces*, 262. PTB Seminar, EUV Metrology, October 27–28, Physikalisch-Technische Bundesanstalt, Berlin, October 28.

116. O. Rott, *An iterative method for the multipliers of periodic delay differential equations*, Brno University of Technology, Department of Machining Technology, Czech Republic, February 16.

117. ———, *Modeling and stability of milling processes*, Technische Universität Berlin, Institut für Mathematik, March 15.

118. J.G.M. Schoenmakers, *New dual methods for single and multiple exercise options*, Workshop “Quantitative Methods in Financial and Insurance Mathematics”, April 18–21, Lorentz Center, Leiden, The Netherlands, April 21.

119. ———, *New dual methods for single and multiple exercise option*, Universität Ulm, Institut für Numerische Mathematik, May 27.

120. ———, *New dual methods for single and multiple exercise options*, International Workshop on Numerical Algorithms in Computational Finance, July 20–22, Goethe Universität Frankfurt, Goethe Center for Scientific Computing, July 22.

121. ———, *Multi-level dual approach for pricing American options*, Workshop on Rough Paths and Numerical Integration Methods, September 21–23, Philipps-Universität Marburg, Fachbereich Mathematik und Informatik, September 23.

122. ———, *Multilevel dual approach for pricing American style derivatives*, University of Oxford, Mathematical Institute, UK, December 1.

123. H. Si, *Tetrahedral mesh generation*, 20th International Meshing Roundtable, October 23–26, Université Pierre et Marie Curie, Paris, France, October 25.

124. V. Spokoiny, *Non-Gaussian component analysis using semi-definite relaxation*, MASCOT NUM (Méthodes d'Analyse Stochastique pour les COdes et Traitements NUMériques) 2011 Workshop, March 23–25, Villard de Lans, France, March 25.

125. ———, *Methods of dimension reduction*, ECONS (Evolving Complex Networks) Spring School and Workshop, March 28–30, Potsdam Institut für Klimafolgenforschung, March 29.

126. ———, *Structure adaptive estimation by alternating*, Workshop "Stuctural Inference Day", April 18, Universität Hamburg, April 18.

127. ———, *Parametric inference. Revisited*, 5èmes Journées Statistiques du Sud, June 14–16, Université Nice Sophia Antipolis, Faculté des Sciences, June 15.

128. ———, *Alternating and semiparametric efficiency*, Conference in Honour of Joel Horowitz, June 23–24, Centre for Microdata Methods and Practice, London, UK, June 24.

129. ———, *Modern parametric theory*, 4 talks, École Nationale de la Statistique et de l'Analyse de l'Information (ENSAI), Rennes, France, September 13–16.

130. ———, *Alternating and semiparametric efficiency*, École Nationale de la Statistique et de l'Analyse de l'Information (ENSAI), Rennes, France, September 16.

131. ———, *Alternating and semiparametric efficiency*, Workshop "Very High Dimensional Semiparametric Models", October 3–7, Mathematisches Forschungsinstitut Oberwolfach, October 4.

132. ———, *Semiparametric estimation alternating and efficiency*, École Nationale de la Statistique et de l'Administration Économique (ENSAE), Paris, France, December 12.

133. J. Sprekels, *Technological and mathematical problems in the industrial growth of semiconductor bulk single crystals*, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, March 15.

134. ———, *Technological and mathematical problems in the industrial growth of semiconductor bulk single crystals*, Workshop "Nonlinear Diffusion: Algorithms, Analysis and Applications", June 6–8, Warwick Mathematics Institute, UK, June 7.

135. ———, *Real-life crystal growth: Turbulence, magnetic fields, heat transfer via radiation, and free boundaries*, Interfaces and Discontinuities in Solids, Liquids and Crystals (INDI2011), Special Session: Between Mechanics and Mathematics: The "Non-smooth" View by Michel Frémond, June 20–23, Gargnano (Brescia), Italy, June 21.

136. ———, *A non-standard phase-field system of Cahn–Hilliard type for diffusive phase segregation*, Schwerpunktkolloquium"Analysis und Numerik", Universität Konstanz, Fachbereich Mathematik und Statistik, July 14.

137. ———, *A nonstandard phase field system of Cahn–Hilliard type for diffusive phase segregation*, Seminario Matematico e Fisico di Milano, Università degli Studi di Milano, Dipartimento di Matematica, Italy, September 21.

138. ———, *Phase field models and hysteresis operators*, Trends in Thermodynamics and Materials Theory 2011, December 15–17, Technische Universität Berlin, December 16.

139. K. Tabelow, *Structural adaptive smoothing fMRI and DTI data*, SFB Research Center "Mathematical Optimization and Applications in Biomedical Sciences", Karl-Franzens-Universität Graz, Institut für Mathematik und Wissenschaftliches Rechnen, Austria, June 8.

140. ———, *Modeling the orientation distribution function by mixtures of angular central Gaussian distributions*, Cornell University, New York, Weill Medical College, USA, June 23.

141. ———, *Diffusion weighted imaging (DTI and beyond) using dti*, The R User Conference 2011, August 15–18, University of Warwick, Department of Statistics, Coventry, UK, August 15.

142. ———, *Functional MRI using fmri*, The R User Conference 2011, August 15–18, University of Warwick, Department of Statistics, Coventry, UK, August 15.

143. ———, *Statistical parametric maps for functional MRI experiments in R: The package fmri*, The R User Conference 2011, August 15–18, University of Warwick, Department of Statistics, Coventry, UK, August 18.

144. ———, *Structural adaptive smoothing fMRI and DTI data*, Maastricht University, Faculty of Psychology and Neuroscience, The Netherlands, September 28.

145. M. Thomas, *Modeling and analysis of rate-independent damage and delamination processes*, 19th International Conference on Computer Methods in Mechanics, Minisymposium "Growth Phenomena and Evolution of Microstructures. Applications in Solids", May 9–12, Warsaw University of Technology, Poland, May 11.

146. ———, *Delamination in viscoelastic materials with thermal effects*, Oberseminar "Mathematik in den Naturwissenschaften", Universität Würzburg, Institut für Mathematik, November 24.

147. V. Tronciu, *Picoseconds pulse amplification — Theory and experiment*, Technical University of Moldova, Department of Physics, Chisinau, April 20.

148. ———, *Nonlinear dynamics in semiconductor lasers — Theory and experiments*, Academy of Sciences of the Republic of Moldova, Institute of Energy, Chisinau, July 28.

149. ———, *Semiconductor lasers — Key elements for chaos based communication systems*, Università di Pavia, Ph.D. School of Electrical and Electronic Engineering and Computer Science, Italy, September 23.

150. ———, *High power lasers for modern technologies*, NANO-2011 Cooperation and Networking of Universities and Research Institutes — Study by Doing Research, October 6–9, Academy of Science, Institute of Electronic Engineering and Nanotechnologies, Kishinev, Moldova, October 8.

151. A.G. Vladimirov, *Synchronization of weakly interacting optical oscillons*, Progress in Electromagnetics Research Symposium, March 20–23, Marrakesh, Morocco, March 23.

152. ———, *Mode-locking in quantum well and quantum dot semiconductor lasers*, Yaroslavl Demidov State University, Russia, August 16.

153. ———, *Delay differential equations model of a mode-locked semiconductor laser*, Yaroslavl Demidov State University, Russia, August 18.

154. ———, *Delay differential equations models in laser dynamics*, Yaroslavl Demidov State University, Russia, August 30.

155. ———, *Cavity solitons in broad area laser systems with delayed feedback*, Yaroslavl Demidov State University, Russia, September 6.

156. B. Wagner, *The role of large slippage during dewetting of polymer solutions from hydrophobised substrates*, 18th Ostwald Kolloquium on "Dynamic Wetting of Complex Liquids", May 16–18, Mainz, May 18.

157. ———, *Nanostrukturierung dünner Filme und ihre Anwendung in der Photovoltaik*, Simulationstreffen (simulation meeting) PVcomB (Competence Centre Thin-Film- and Nanotechnology for Photovoltaics Berlin), Technische Universität Berlin, November 3.

158. W. Wagner, *Direct simulation Monte Carlo algorithms*, Università di Catania, Dipartimento di Matematica e Informatica, Italy, October 6.

159. L. Wilhelm, *An abstract Landauer–Büttiker formula with application to a toy model of a quantum dot LED*, Analysis Seminar, Aalborg University, Department of Mathematical Sciences, Denmark, June 16.

160. T. Wolff, *Random walk among random conductances*, Spring Meeting Beijing/Bielefeld — Berlin/Zurich of the International Research Group Stochastic Models of Complex Processes, March 30 – April 1, Technische Universität Berlin, March 31.

161. ———, *The parabolic Anderson model from the perspective of a moving catalyst*, 7th Cornell Probability Summer School, July 8–24, Cornell University, Ithaka, USA, July 18.

162. ———, *Annealed behaviour of local times in the random conductance model*, 2011 School on Mathematical Statistical Physics, September 4–9, Charles University of Prague, Center for Theoretical Study, and Academy of Sciences of the Czech Republic, Institute of Theoretical Computer Science, September 8.

163. M. Wolfrum, *Stability properties of equilibria and periodic solutions in systems with large delay*, Equadiff 2011, August 1–5, University of Loughborough, UK, August 2.

164. ———, *Stability properties of equilibria and periodic solutions in systems with large delay*, The Sixth International Conference on Differential and Functional Differential Equations (DFDE 2011), August 17–21, Steklov Mathematical Institute, Moscow, Russia, August 19.

165. ———, *Mechanisms of semi-strong pulse interaction in the Schnakenberg model*, Seminar z kvalitativnej teorie diferencialnych rovnic, Comenius University, Bratislava, Slovakia, November 10.

166. J. Zhang, *Solvability and numerical simulation of BSDEs related to BSPDEs with applications to utility maximization*, Universität Innsbruck, Fachbereich Mathematik, Austria, April 26.

167. ———, *Lp-solutions of BSDEs with time delayed generators*, Mathematikkolloquium, Universität Innsbruck, Fachbereich Mathematik, Austria, April 28.

A.8.3 Talks for a More General Public

1. U. Bandelow, *Schwarze Löcher im Labor*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2011, WIAS, May 28.
2. E. Diederichs, *Schönheitskriterien unter Hühnern*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2011, WIAS, May 28.
3. C. Guhlke, *Ein Fall für die Mathematik*, Matheon Rent the Center, Primo-Levi-Schule, Berlin, January 25.
4. ———, *Luftballons, Wasserstoffautos und Lithium-Ionen-Batterien — Unmögliches zusammenbringen, das schafft nur die Mathematik!*, 16. Berliner Tag der Mathematik (16th Berlin Day of Mathematics), Beuth Hochschule für Technik Berlin, May 7.
5. ———, *Luftballons, Lithium-Ionen-Batterien und Wasserstoffautos — Ein Fall für die Mathematik*, Matheon Rent the Center, KLAX-Sekundarschule, Berlin, December 19.
6. R. Henrion, *Der optimierte Zufall*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2011, WIAS, May 28.
7. S. Jachalski, D. Peschka, *Wundersame Flüssigkeiten*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2011, WIAS, May 28.

8. W. KÖNIG, *Die Anfänge der Wahrscheinlichkeitsrechnung als Wissenschaft*, 2 talks, Lange Nacht der Wissenschaften (Long Night of the Sciences) 2011, WIAS, May 28.

9. ———, *Streifzüge durch die Entwicklung der Wahrscheinlichkeitsthorie*, Goethe-Gymnasium Potsdam, June 28.

10. ———, *Erfolgsgeschichte eines stochastischen Prozesses: Die Brown'sche Bewegung*, Weinberg-Gymnasium Kleinmachnow, November 17.

11. ———, *Streifzüge durch die Entwicklung der Wahrscheinlichkeitsthorie*, 2 talks, Weinberg-Gymnasium Kleinmachnow, November 17.

12. M. LIERO, *Mathematik und Solarzellen*, 16. Berliner Tag der Mathematik (16th Berlin Day of Mathematics), Beuth Hochschule für Technik Berlin, May 7.

13. A. MIELKE, *0 durch 0 oder Grenzschichten in der Photovoltaik*, MathInside — Mathematik ist überall, Urania, Berlin, March 22.

14. K. TABELOW, *Geschärfte Blicke in das Gehirn*, MathInside — Mathematik ist überall, Urania, Berlin, January 18.

15. ———, *Geschärfte Blicke in das Gehirn*, Festveranstaltung zum 50jährigen Jubiläum des Heinrich-Hertz-Gymnasiums, September 23.

16. ———, *Mathematik in der Gehirnforschung — Von der Formel zur Erkenntnis*, Mathematik und Gesundheit, MATHEON and Urania, Berlin, September 26.

17. M. THOMAS, *Vom Hooke'schen Gesetz zu schlauen Materialien*, 16. Berliner Tag der Mathematik (16th Berlin Day of Mathematics), Beuth-Hochschule für Technik Berlin, May 7.

A.8.4 Posters

1. S. AMIRANASHVILI, *Optical transistor: From optical event horizons to rogue waves*, Rogue Waves, Dresden, November 7–11.

2. A. CAIAZZO, *Atlas-based fast patient-specific simulations of the pulmonary artery*, 2nd International Conference on Engineering Frontiers in Congenital Heart Disease, London, UK, March 17–18.

3. A. CAIAZZO, J. FUHRMANN, V. JOHN, *Finite element-finite volume coupling for simulations of thin porous layer fuel cells*, Workshop on Simulation of Flow in Porous Media and Applications in Waste Management and CO2 Sequestration, John Radon Institute for Computational and Applied Mathematics, Linz, Austria, October 3–7.

4. A. FIEBACH, K. GÄRTNER, *Finite-volume-approximation of the Michaelis–Menten kinetics*, 3rd Spring School "Analytical and Numerical Aspects of Evolution Equations", Essen, March 28 – April 1.

5. J. FUHRMANN, H. ZHAO, H. LANGMACH, *Numerical modeling of CO oxidation on Pt surfaces coupled with convective mass transport*, XXXI Dynamics Days Europe 2011, Oldenburg, September 12–16.

6. K. GÄRTNER, *Charge transport in semiconductors and a finite volume scheme*, Finite Volumes for Complex Applications VI (FVCA 6), Prague, Czech Republic, June 6.

7. A. GLITZKY, J.A. GRIEPENTROG, *Discrete Sobolev–Poincaré inequalities for Voronoi finite volume approximations*, Finite Volumes for Complex Applications VI (FVCA 6), Prague, Czech Republic, June 6–10.

8. O. KLEIN, *Representation of hysteresis operators for vector-valued inputs by functions on strings*, International Symposium on Hysteresis Modelling and Micromagnetics (HMM 2011), Levico (Trento), Italy, May 9–11.

9. D. PESCHKA, *Structure formation in thin liquid films*, Workshop on Phase Field Models in Fluid Mechanics, Regensburg, February 14–16.

10. M. Radziunas, K. Staliunas, *Spatial "rocking" in broad area semiconductor lasers*, European Semiconductor Laser Workshop (ESLW) 2011, Lausanne, Switzerland, September 23–24.
11. K. Tabelow, S. Keller, S. Mohammadi, H. Kugel, J.-S. Gerdes, J. Polzehl, M. Deppe, *Structural adaptive smoothing increases sensitivity of DTI to detect microstructure alterations*, 17th Annual Meeting of the Organization on Human Brain Mapping (HBM 2011), Quebec City, Canada, June 26–30.
12. K. Tabelow, H. Voss, J. Polzehl, *Package dti: A framework for HARDI modeling in R*, 17th Annual Meeting of the Organization on Human Brain Mapping (HBM 2011), Quebec City, Canada, June 26–30.
13. ———, *Structural adaptive smoothing methods for fMRI and its implementation in R*, 17th Annual Meeting of the Organization on Human Brain Mapping (HBM 2011), Quebec City, Canada, June 26–30.
14. K. Tabelow, B. Whitcher, J. Polzehl, *Performing tasks in medical imaging with R*, 17th Annual Meeting of the Organization on Human Brain Mapping (HBM 2011), Quebec City, Canada, June 26–30.
15. V.Z. Tronciu, M. Radziunas, S. Schwertfeger, A. Klehr, U. Bandelow, H. Wenzel, *Modelling of dynamics in broad area semiconductor devices: Picosecond pulse amplification in tapered amplifiers*, European Semiconductor Laser Workshop (ESLW) 2011, Lausanne, Switzerland, September 23–24.
16. A. Wilms, A. Schliwa, Th. Koprucki, D. Breddermann, P. Mathé, A. Knorr, U. Bandelow, *Theory of Coulomb scattering from two- and three-dimensional reservoirs to quantum dot states*, 11th International Conference on Physics of Light-Matter Coupling in Nanostructures (PLMCN11), Berlin, April 6.

A.9 Visits to other Institutions[6]

1. R. Arkhipov, CNRS Laboratory for Photonics and Nanostructures and III-IV LAB, Marcoussis (Paris), France, November 23–26.
2. U. Bandelow, Australian National University (ANU), Research School of Physics and Engineering, Canberra, November 30, 2011 – January 24, 2012.
3. J. Borchardt, ALSTOM Power, Baden, Switzerland, June 6–11.
4. A. Caiazzo, Institut National de Recherche en Informatique et Automatique (INRIA), REO, Paris, France, July 7–15.
5. W. Dreyer, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, February 28 – March 4.
6. G. Faraud, Université de Brest, Laboratoire de Mathématiques, France, June 16–26.
7. ———, Université Paris VI "Pierre et Marie Curie", Laboratoire de Probabilités et Modèles Aléatoires, France, November 18–25.
8. K. Gärtner, Universität Basel, Institut für Informatik, Switzerland, August 1–14.
9. ———, Guest Professorship, King Abdullah University of Science and Technology, Saudi Arabia, September 1 – December 31.
10. O. Gün, Université de Provence, Marseille, France, May 30 – June 25.
11. ———, Rheinische Friedrich-Wilhelms-Universität Bonn, Institut für Angewandte Mathematik, December 2–8.
12. D. Hömberg, Nippon Steel Science Forum, University of Oxford, Oxford Centre for Industrial and Applied Mathematics, UK, January 11–15.
13. ———, Southeast University, Department of Mathematics, Nanjing, Republic of China, March 23–28.
14. ———, Fudan University, School of Mathematics, Shanghai, Republic of China, March 29 – April 3.
15. ———, Università degli Studi di Milano, Dipartimento di Matematica "F. Enriques", Italy, November 8–12.
16. ———, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche, Pavia, Italy, November 13–17.
17. G. Hu, Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria, November 26 – December 2.
18. S. Jansen, The University of Arizona, Department of Mathematics, Tucson, USA, April 8 – June 19.
19. ———, Université de Nice Sophia-Antipolis, Département de Mathématiques, France, July 25 – August 31.
20. ———, University of Warwick, Department of Mathematics, UK, November 10–18.
21. V. John, Universidad Autónoma de Madrid, Departamento de Matemáticas, Spain, March 7–11.
22. ———, Univerity of Pittsburg, Department of Mathematics, USA, May 16–27.
23. ———, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, June 20–24.
24. D. Knees, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, February 28 – March 3.
25. ———, Università degli Studi di Udine, Dipartimento di Matematica e Informatica, Italy, March 6–11.

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

26. ———, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche, Pavia, Italy, November 29 – December 2.
27. W. König, University of Warwick, Mathematics Institute, Coventry, UK, February 15–24.
28. ———, University of California at Los Angeles, Department of Mathematics, USA, March 31 – April 18.
29. ———, Universität Zürich, Institut für Mathematik, Switzerland, June 5–10.
30. ———, Tokyo Institute of Technology, Department of Mathematics, Japan, November 30 – December 10.
31. Ch. Kraus, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, May 2–6.
32. M. Liero, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche, Pavia, Italy, October 10–14.
33. A. Linke, Clemson University, Department of Mathematical Sciences, USA, July 23–29.
34. R.L. Loeffen, University of Wroclaw, Faculty of Mathematics and Computer Science, Poland, May 12 – June 3.
35. A. Mielke, Università di Pavia, Dipartimento di Matematica, Italy, March 28 – April 1.
36. ———, Charles University, Mathematical Institute, Prague, Czech Republic, September 26–30.
37. H. Neidhardt, Aalborg University, Department of Mathematical Sciences, Denmark, June 14–18.
38. ———, Université Aix-Marseille 2, Centre de Physique Théorique, France, November 2–13.
39. O. Omel'chenko, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, January 30 – February 6.
40. ———, Drexel University, Department of Mathematics, Philadelphia, USA, May 27–31.
41. D. Peschka, Department of Mathematics, University of California, Los Angeles, USA, October 17 – November 11.
42. Th. Petzold, Nippon Steel Science Forum, University of Oxford, Oxford Centre for Industrial and Applied Mathematics, UK, January 11–15.
43. J. Polzehl, University of Minnesota, School of Statistics, USA, June 1–25.
44. M. Radziunas, CNRS Laboratory for Photonics and Nanostructures and III-IV LAB, Marcoussis (Paris), France, November 23–26.
45. V. Schlosshauer, ALSTOM Power, Baden, Switzerland, June 6–9.
46. V. Spokoiny, École Nationale de la Statistique et de l'Analyse de l'Information (ENSAI), Rennes, France, September 13–16.
47. ———, Russian Academy of Sciences, Institute for Information Transmission Problems (Kharkevich Institute), Moscow, October 30 – November 2.
48. ———, École Nationale de la Statistique et de l'Analyse de l'Information (ENSAI), Rennes, France, November 3–17.
49. J. Sprekels, Università di Pavia, Dipartimento di Matematica "F. Casorati", Italy, September 19–24.
50. K. Tabelow, Cornell University, Weill Medical College, New York, USA, June 22–25.
51. M. Thomas, Università di Pavia, Dipartimento di Matematica, Italy, June 13–18.
52. ———, Università di Brescia, Dipartimento di Matematica, Italy, November 2–6.
53. V. Tronciu, Academy of Sciences of Moldova, Chisinau, July 25–29.

54. ———, University of Pavia, School of Electrical and Electronic Engineering and Computer Science, Italy, September 21–25.
55. A.G. Vladimirov, Tyndall National Institute, Cork, Ireland, March 6–9.
56. ———, Yaroslavl Demidov State University, Russia, August 14–21.
57. ———, Yaroslavl Demidov State University, Russia, August 29 – September 9.
58. ———, CNRS Laboratory for Photonics and Nanostructures and III-IV LAB, Marcoussis (Paris), France, November 23–26.
59. W. Wagner, Università di Catania, Dipartimento di Matematica e Informatica, Italy, October 4–11.
60. L. Wilhelm, Aalborg University, Department of Mathematical Sciences, Denmark, June 14–18.
61. M. Wolfrum, National Academy of Sciences of Ukraine, Institute of Mathematics, Kiev, January 30 – February 6.
62. ———, Comenius University, Department of Applied Mathematics and Statistics, Bratislava, Slovakia, November 7–11.
63. J. Zhang, Universität Innsbruck, Fachbereich Mathematik, Austria, April 26 – May 2.

A.10 Academic Teaching[7]

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. W. König, *Große Abweichungen* (seminar), Technische Universität Berlin, 4 SWS.
19. J. Blath, J. Gärtner, W. König, N. Kurt, *Stochastic Models in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 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.

[7] SWS = semester periods per week

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.

Summer Semester 2011

1. P. Friz, *Stochastik und Finanzmathematik* (practice), Technische Universität Berlin, 2 SWS.
2. L. Recke, H.-J. Wünsche, U. Bandelow, *Mathematische Modelle der Photonik* (research seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
3. M. Becker, *Wahrscheinlichkeitstheorie für Lehramt* (seminar), Universität Leipzig, 2 SWS.
4. R. Henrion, W. Römisch, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
5. D. Hömberg, *Differentialgleichungen für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS.
6. S. Jansen, *Mathematics for Engineers, Master Program: Global Productions Engineering* (lecture), Technische Universität Berlin, 2 SWS.
7. ———, *Mathematics for Engineers, Master Program: Global Productions Engineering* (practice), Technische Universität Berlin, 2 SWS.
8. 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.
9. O. Klein, *Optimale Steuerung partieller Differentialgleichungen I* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
10. J. Blath, J. Gärtner, W. König, N. Kurt, *Stochastic Models in Physics and Biology* (senior seminar), Technische Universität Berlin, 2 SWS.
11. J.-D. Deuschel, P. Friz, J. Gärtner, P. Imkeller, W. König, U. Küchler, H. Föllmer, *Berliner Kolloquium Wahrscheinlichkeitstheorie* (seminar), WIAS Berlin, 2 SWS.
12. Ch. Kraus, *Allgemeine Variationsmethoden II* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
13. K. Krumbiegel, *Analysis I für Ingenieure* (lecture), Technische Universität Berlin, 4 SWS.
14. P. Mathé, *Computational Statistics (CoSta)* (lecture), Freie Universität Berlin, 2 SWS.
15. A. Mielke, *Höhere Analysis II: Partielle Differentialgleichungen/BMS Basic Course "Partial Differential Equations"* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
16. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin, 2 SWS.
17. V. Spokoiny, *Nichtparametrische Methoden* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
18. V. Spokoiny, W. Härdle, M. Reiss, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
19. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.

20. M. Wolfrum, B. Fiedler, St. Liebscher, *Nonlinear Dynamics* (senior seminar), WIAS Berlin/Freie Universität Berlin, 2 SWS.

Winter Semester 2011/2012

1. P. Friz, *Stochastik und Finanzmathematik* (practice), Technische Universität Berlin, 2 SWS.
2. ———, *Differential Equations for Probabilists* (lecture seminar), Technische Universität Berlin, 4 SWS.
3. M. Becker, *Grundwissen Schulmathematik* (seminar), Universität Leipzig, 2 SWS.
4. J. Fuhrmann, *Differentialgleichungen für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS.
5. A. Glitzky, *Einführung in die Kontrolltheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
6. R. Henrion, *Optimierungsprobleme mit Wahrscheinlichkeitsrestriktionen* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
7. R. Henrion, W. Römisch, *Numerik stochastischer Modelle* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
8. D. Hömberg, *Integraltransformationen und partielle Differentialgleichungen für Ingenieure* (lecture), Technische Universität Berlin, 2 SWS.
9. V. John, *Numerik IVb: Simulation und Optimierung von Prozessen aus der Strömungsmechanik* (lecture), Freie Universität Berlin, 2 SWS.
10. ———, *Numerik IVb: Simulation und Optimierung von Prozessen aus der Strömungsmechanik* (seminar), Freie Universität Berlin, 2 SWS.
11. ———, *Numerik IVb: Simulation und Optimierung von Prozessen aus der Strömungsmechanik* (practice), Freie Universität Berlin, 2 SWS.
12. 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.
13. O. Klein, *Optimale Steuerung partieller Differentialgleichungen II* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
14. D. Knees, *Nichtlineare partielle Differentialgleichungen/BMS Advanced Course "Nonlinear Partial Differential Equations"* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
15. 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.
16. Ch. Kraus, *Variationsrechnung* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
17. A. Linke, *Mathematik für Physiker I* (seminar), Freie Universität Berlin, 4 SWS.
18. ———, *Mathematik für Physiker I* (practice), Freie Universität Berlin, 2 SWS.
19. A. Mielke, *Höhere Analysis I (Funktionalanalysis)/BMS Basic Course "Functional Analysis"* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
20. H. Gajewski, A. Mielke, J. Sprekels, *Nichtlineare partielle Differentialgleichungen (Langenbach-Seminar)* (senior seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
21. L. Recke, H.-J. Wünsche, M. Radziunas, *Mathematische Modelle der Photonik* (research seminar), WIAS Berlin/Humboldt-Universität zu Berlin, 2 SWS.
22. J.G.M. Schoenmakers, *Monte Carlo basierte Methoden in der Finanzmathematik* (lecture), Humboldt-Universität zu Berlin, 2 SWS.

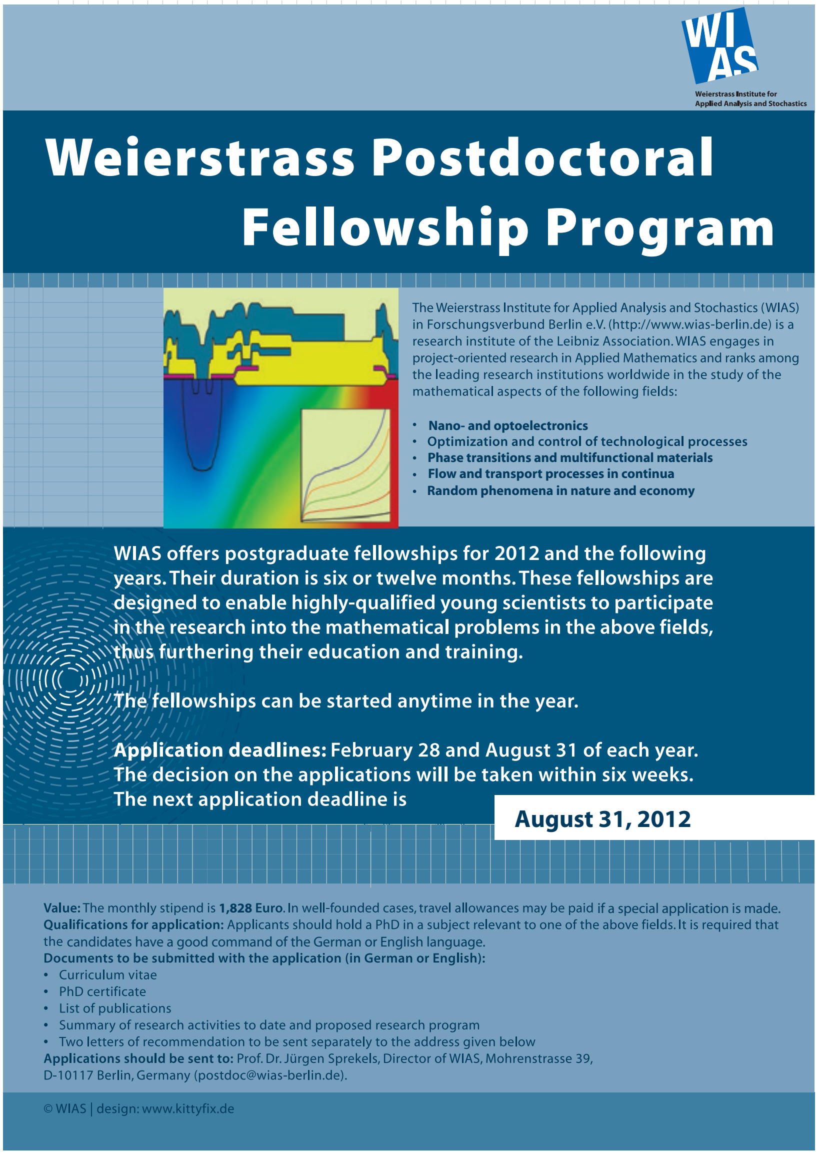
23. V. Spokoiny, *Nichtparametrische Verfahren* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
24. V. Spokoiny, W. Härdle, M. Reiss, *Mathematical Statistics* (seminar), Humboldt-Universität zu Berlin, 2 SWS.
25. J. Sprekels, *Analysis I* (lecture), Humboldt-Universität zu Berlin, 4 SWS.
26. H. Stephan, *Anfänge der Algebra und Gleichungstheorie* (lecture), Humboldt-Universität zu Berlin, 2 SWS.
27. K. Tabelow, *Mathematik* (seminar), Steinbeis Hochschule Berlin, 2 SWS.
28. 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.

In 2011, Dr. Matthew Roberts (Université Pierre et Marie Curie (Paris VI), France), Dr. Natalia Bochkina (Edinburgh University, UK), and Dr. Karoline Götze (Technische Universität Darmstadt) worked as fellowship holders at WIAS.



A.12 Visiting Scientists[8]

A.12.1 Guests

1. St. Adams, University of Warwick, Mathematics Institute, Coventry, UK, September 11–18.
2. D.A. Arroyo Almanza, Universidad de Palma de Mallorca, Instituto de Física Interdisciplinar y Sistemas Complejos, Spain, May 30 – June 3.
3. G.R. Barrenechea, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, August 28 – September 4.
4. Ch. Bayer, Universität Wien, Fakultät für Mathematik, Austria, February 7–10.
5. M. Biskup, University of California, Los Angeles, Department of Mathematics, USA, August 8–12.
6. ———, August 22–26.
7. ———, December 12–16.
8. M. Bogomolov, Tel Aviv University, School of Mathematical Sciences, Israel, June 3–7.
9. E. Bonetti, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, May 16–20.
10. J. Bradic, Princeton University, Department of Operations Research and Financial Engineering, USA, March 20 – April 21.
11. K. Chełminski, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, August 22 – September 2.
12. ———, November 21–25.
13. X. Chen, Yale University, Department of Economics, New Haven, USA, June 6–12.
14. R. Ciegis, Gediminas Technical University, Department of Mathematical Modeling, Vilnius, Lithuania, November 28 – December 10.
15. P. Colli, Università di Pavia, Dipartimento di Matematica, Italy, February 6–18.
16. W. de Roeck, Universität Heidelberg, Institut für Theoretische Physik, July 13–16.
17. R. Eymard, Université Paris Est, Département de Mathématiques, Marne-la-Vallée, France, January 11–14.
18. L.A. Fernandez, Universidad de Cantabria, Departamento de Matémáticas, Santander, Spain, November 21–27.
19. A. Fiaschi, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche, Pavia, Italy, May 3–7.
20. F. Gach, University of Cambridge, Department of Mathematics, UK, February 8–13.
21. M. Gerdts, Universität der Bundeswehr München, Institut für Mathematik und Rechneranwendung, Neubiberg, August 15 – September 12.
22. G. Gilardi, Università di Pavia, Dipartimento di Matematica, Italy, February 6–11.
23. D. Glyzin, Yaroslavl State University, Department Modeling and Analysis of Information Systems, Russia, November 28 – December 4.
24. M. Grasselli, Politecnico di Milano, Dipartimento di Matematica, Italy, May 1–6.

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

25. A. Grin, State University of Grodno, Faculty of Mathematics and Informatics, Belarus, December 10–14.
26. M. Grmela, École Polytechnique de Montréal, Department of Chemical Engineering, Canada, July 12–15.
27. R. Haller-Dintelmann, Technische Universität Darmstadt, Fachbereich Mathematik, December 12–16.
28. M.-L. Hein, Freie Universität Berlin, Fachbereich Mathematik, August 29 – September 30.
29. M. Hirokawa, Okayama University, Graduate School of Natural Sciences and Technology, Department of Mathematics, Japan, August 28 – September 23.
30. B. Hofmann, Technische Universität Chemnitz, Fakultät für Mathematik, March 14–18.
31. M. Hoyuelos, Universidad Nacional de Mar del Plata, Facultad de Ciencias Exactas y Naturales, Argentina, February 27 – March 16.
32. G. Huyet, Cork Institute of Technology, Physics Department, Ireland, June 27 – July 8.
33. A. Jourani, Université de Bourgogne, Département de Mathématiques, Dijon, France, September 4–18.
34. A. Juditsky, Université Joseph Fourier Grenoble I, Laboratoire de Modélisation et Calcul, France, April 24 – May 2.
35. P. Jung, Sogang University, Department of Mathematics, Seoul, Korea, June 29 – July 25.
36. P. Knobloch, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, August 14 – September 1.
37. Th. Kolokolnikov, Dalhousie University, Mathematics and Statistics Department, Halifax, Canada, August 8–13.
38. V. Koltchinski, Georgia Institute of Technology, School of Mathematics, Atlanta, USA, April 11 – March 30.
39. D. Kourounis, Stanford University, Department of Energy Resources Engineering, USA, June 19–22.
40. H. Kovarik, Politecnico di Torino, Dipartimento di Matematica, Italy, September 12–16.
41. M. Kraft, University of Cambridge, Department of Chemical Engineering, UK, January 3–8.
42. ———, July 25 – August 19.
43. P. Krejčí, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, October 31 – November 11.
44. C. Laing, Massey University, Institute of Information and Mathematical Sciences, Auckland, New Zealand, November 21–27.
45. Ch. Lenglet, University of Minnesota, Medical School, Minneapolis, USA, November 21–26.
46. O. Lepski, Université de Provence, Centre de Mathématiques et Informatique, Marseille, France, May 8, 2010 – May 17, 2011.
47. J. Liu, Southeast University, Department of Mathematics, Nanjing, Republic of China, September 11–20.
48. Q. Liu, Universität Bremen, Institut für Technomathematik, May 2–27.
49. V.L. Maistrenko, National Academy of Sciences of Ukraine, National Scientific Centre for Medical and Biotechnical Research, Kiev, August 7–14.
50. Y. Maistrenko, Academy of Sciences of Ukraine, National Scientific Centre for Medical and Biotechnical Research, Kiev, September 24 – October 1.
51. M.M. Malamud, Donetsk National University, Department of Mathematics, Ukraine, February 13–16.
52. M. Malioutov, Northeastern University, Department of Mathematics, Boston, USA, February 22 – March 21.

53. ———, August 24–29.
54. ———, September 2–6.
55. P.A. Markowich, Cambridge University, Department of Applied Mathematics and Theoretical Physics, UK, and University of Vienna, Faculty of Mathematics, Austria, June 20 – July 1.
56. M. Matviichuk, National Taras Sevchenko University of Kiev, Institute of Mathematics, Ukraine, February 14 – March 15.
57. N. McCullen, University of Leeds, School of Mathematics, UK, December 11–18.
58. M. Meyries, Karlsruher Institut für Technologie, Institut für Analysis, December 5–8.
59. G.L. Miller, Carnegie Mellon University, Computer Science Department, Pittsburgh, USA, June 16–19.
60. G. Milstein, Ural State University, Institute of Physics and Applied Mathematics, Ekaterinburg, Russia, August 22 – October 21.
61. S. Mohammed, Southern Illinois University, Department of Mathematics, USA, July 25 – August 28.
62. A. Münch, University of Oxford, Oxford Center for Industrial and Applied Mathematics, Mathematical Institute, UK, March 10–15.
63. ———, March 18–24.
64. ———, June 24–29.
65. ———, July 10–15.
66. O. Muscato, Università degli Studi di Catania, Dipartimento di Matematica e Informatica, Italy, July 31 – August 7.
67. J. Nakagawa, Nippon Steel Corporation, Tokyo, Japan, January 17–20.
68. J. Novo, Universidad Autonoma de Madrid, Instituto de Ciencias Matemáticas, Madrid, Spain, October 31 – November 4.
69. J. Outrata, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, September 5–12.
70. L. Paoli, Université de Saint-Etienne, Laboratoire de Mathématiques, France, January 4 – February 15.
71. ———, May 30 – June 17.
72. V. Patilea, Ecole Nationale de la Statistique et de l'Analyse de l'Information, Campus de Ker-Lann, Bruz, France, May 29 – June 3.
73. I. Popov, St.-Petersburg State University of Information Technologies, Mechanics and Optics, Department of Higher Mathematics, Russia, January 31 – February 6.
74. R. Purice, Simion Stoilow Institute of Mathematics of the Romanian Academy, Bucharest, Romania, February 1–4.
75. M.G. Rasmussen, Aarhus University, Department of Mathematical Sciences, Denmark, March 20 – April 5.
76. P. Reynaud-Bouret, Université de Nice Sophia-Antipolis, Laboratoire de Mathématiques J.A. Dieudonné, France, July 10–16.
77. E. Rocca, Università degli Studi di Milano, Dipartimento di Matematica "F. Enriques", Italy, February 7–11.
78. Th. Roche, Technische Universität München, Fakultät für Mathematik, May 26 – June 2.
79. R. Rossi, Università di Brescia, Dipartimento di Matematica, Italy, February 21–25.
80. ———, May 23 – June 4.

81. ———, September 8–24.

82. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, January 24 – February 23.

83. ———, August 22 – September 21.

84. A. Segatti, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, May 16–20.

85. Y. Shao, Hochschule Zittau-Görlitz, Fakultät Mathematik-Naturwissenschaften, November 14–18.

86. J. Shewchuk, University of California at Berkeley, Computer Science Division, USA, August 23 – September 14.

87. D. Skovmand, Aarhus University, Department of Business Studies, Denmark, February 20–25.

88. J. Sokołowski, Université de Nancy 1, Laboratoire de Mathématiques, Vandœuvre-lès-Nancy, France, August 18–22.

89. O.O. Sudakov, National Academy of Sciences of Ukraine, National Centre for Medical and Biotechnical Research, Kiev, March 20 – April 3.

90. A. Torcini, Institute for Complex Systems, Florence, Italy, February 15–19.

91. H. Tran, University of Pittsburgh, Mathematics, USA, November 20 – December 18.

92. M. Tretyakov, University of Leicester, Department of Mathematics, UK, September 12–23.

93. D. Turaev, Imperial College London, Department of Mathematics, UK, July 17 – August 4.

94. D. Ueltschi, University of Warwick, Department of Mathematics, UK, December 12–19.

95. A. Vasylenko, National Scientific Centre for Biotechnical Research, Kiev, Ukraine, August 7–21.

96. Th. Wagenknecht, University of Leeds, Department of Applied Mathematics, UK, December 11–16.

97. L. Wissler, Freie Universität Berlin, Fachbereich Informatik, July 20 – September 2.

98. M. Yamamoto, University of Tokyo, Department of Mathematical Sciences, Japan, January 17–20.

99. ———, March 9–28.

100. ———, September 9–30.

101. M. Yvinec, Institut National de Recherche en Informatique et en Automatique (INRIA), Geometrica project team, France, May 22–28.

102. Ch. Zanini, Università degli Studi di Udine, Dipartimento di Matematica e Informatica, Italy, April 18–22.

103. S. Zelik, University of Surrey, Faculty of Engineering and Physical Sciences, Department of Mathematics, Guildford, UK, December 9–24.

A.12.2 Scholarship Holders

1. S. Becker, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, Promotionsstipendium (doctoral scholarship), Stiftung der Deutschen Wirtschaft e. V., September 1, 2010 – February 28, 2013.

2. N. Berger, The Hebrew University of Jerusalem, Einstein Institute of Mathematics, Faculty of Sciences, Israel, Humboldt Research Fellowship, September 1, 2010 – August 31, 2011.

3. N. Bochkina, Edinburgh University, School of Mathematics, UK, Weierstrass Postdoctoral Fellowship Program, April 15 – July 15.

4. P. Friz, Technische Universität Berlin, Institut für Mathematik, WIAS, June 12, 2009 – June 11, 2014.

5. S. Ganesan, Indian Institute of Science, Supercomputer Education and Research Centre, Bangalore, Humboldt Research Fellowship, May 1, 2010 – June 15, 2011.
6. K. Götze, Technische Universität Darmstadt, Fachbereich Mathematik, Weierstrass Postdoctoral Fellowship Program, September 1, 2011 – January 31, 2012.
7. S. Lu, Fudan University, School of Mathematical Sciences, Shanghai, China, Humboldt Research Fellowship, September 12, 2011 – September 1, 2012.
8. M. Roberts, Université Pierre et Marie Curie (Paris VI), Laboratoire de Probabilités, Paris, France, Weierstrass Postdoctoral Fellowship Program, January 1 – June 30.
9. U. Stefanelli, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche, Pavia, Italy, Friedrich Wilhelm Bessel Research Award by Alexander von Humboldt Foundation, March 1 – July 31.

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

1. B. Bugert, Berlin Mathematical School, doctoral candidate, December 1, 2010 – December 1, 2012.
2. 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.
3. C. Patz, Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, doctoral candidate, March 1, 2009 – September 11, 2013.
4. M. Salvi, Technische Universität Berlin, International Research Training Group GRK 1339: “Stochastic Models of Complex Systems and Their Applications”, doctoral candidate, April 1, 2010 – March 31, 2012.
5. A. Schnitzler, Technische Universität Berlin, International Research Training Group GRK 1339: “Stochastic Models of Complex Systems and Their Applications”, doctoral candidate, April 1, 2010 – December 31, 2011.
6. W. Wang, Humboldt-Universität zu Berlin, Wirtschaftswissenschaftliche Fakultät, doctoral candidate, October 1, 2009 – March 31, 2012.
7. U. Wilbrandt, Freie Universität Berlin, Institut für Mathematik, Helmholtz-Kolleg GEOSIM, doctoral candidate, October 1, 2011 – September 30, 2013.

A.13 Guest Talks

1. St. Adams, University of Warwick, Mathematics Institute, Coventry, UK, *Random field of gradients*, September 14.
2. N. Ahmed, Otto-von-Guericke Universität Magdeburg, Institut für Analysis und Numerik, *Operator splitting and alternating direction Galerkin methods applied to population balance equation*, January 20.
3. S. Alonso, Physikalisch-Technische Bundesanstalt Berlin, *Effective medium theory for randomly heterogeneous reaction-diffusion media*, October 19.
4. A. Andresen, Humboldt-Universität zu Berlin, Institut für Mathematik, *Schilder's theorem for Hilbert space valued Wiener processes, a sequence space approach*, July 12.
5. R. Arkhipov, Saint-Petersburg State University, Department of Optics, Russia, *Theoretical investigations of some problems interaction of resonance laser radiation and matter — Analytical and numerical simulations*, July 19.
6. S. Athreya, Indian Statistical Institute, Bangalore, *Brownian motion on R trees*, June 29.
7. G.R. Barrenechea, University of Strathclyde, Department of Mathematics and Statistics, Glasgow, UK, *Computable error bounds and an adaptive selection of the stabilization parameter for the Stokes problem*, September 1.
8. Ch. Bayer, Universität Wien, Fakultät für Mathematik, Austria, *Some applications of cubature on Wiener space*, February 8.
9. M. Becker, Leibniz-Institut für Plasmaforschung und Technologie e.V., Greifswald, *Hydrodynamische Modelle und numerische Verfahren zur Beschreibung von Niedertemperaturplasmen*, December 19.
10. M. Biskup, University of California, Los Angeles, Department of Mathematics, USA, *A CLT without local CLT in random conductance models with heavy lower tails*, August 22.
11. N. Bochkina, University of Edinburgh, School of Mathematics, UK, *Consistency and efficiency of the posterior distribution in generalised linear inverse problems*, May 10.
12. M. Bogomolov, Tel Aviv University, School of Mathematical Sciences, Israel, *Hierachical testing of subsets of hypotheses*, June 7.
13. Th. Böhme, IAV GmbH — Ingenieurgesellschaft Auto und Verkehr, *Herausforderungen der Elektrifizierung von PkW-Antriebssträngen — Regelungstechnische Ansätze und Methoden*, November 28.
14. E. Bonetti, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, *Dissipation in domains and on interfaces*, May 19.
15. J. Bradic, Princeton University, Department of Operations Research and Financial Engineering, USA, *Regularization for Cox's proportional hazards models with NP dimensionality*, April 13.
16. M. Brokate, Technische Universität München, Zentrum Mathematik M6, Garching, *Optimal control of ODE systems involving a variational inequality*, October 11.
17. Y. Chang, Indiana University, Department of Economics, Bloomington, USA, *Nonstationarity in time series of state densities*, December 7.
18. K. Chełminski, Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland, *Poroplasticity with Cosserat effects*, September 1.
19. ———, *New results in the theory of inelastic deformations*, November 22.
20. X. Chen, Yale University, Department of Economics, New Haven, USA, *On inference of PSMD estimators of semi/nonparametric conditional moment models*, June 8.

21. V. Chernozukov, Massachusetts Institute of Technology, Department of Economics, USA, *Intersection bounds: Estimation and inference*, July 6.

22. R. Ciegis, Gediminas Technical University, Department of Mathematical Modeling, Vilnius, Lithuania, *Numerical approximation of one model of the bacterial self-organization: Analysis of the dynamics*, December 8.

23. X. Claeys, L'Institut Supérieur de l'Aéronautique et de l'Espace, Département Mathématiques, Informatique, Automatique, Toulouse, France, *Integral formulation of the second kind for multi-subdomain scattering*, July 13.

24. P. Colli, Università di Pavia, Dipartimento di Matematica, Italy, *Solutions to models of phase segregation — Part 1*, February 6.

25. S. Eichstädt, Physikalisch-Technische Bundesanstalt Berlin, Arbeitsgruppe 8.41 Modellierung und Simulation, *Statistische Methoden zur Analyse dynamischer Messungen*, January 18.

26. G. Eisenstein, Technion — Israel Institute of Technology, Haifa, *Ultrafast phenomena in quantum dot/dash gain media: From instanteneous gain to two photon induced lasing*, June 16.

27. Ch. Elliott, University of Warwick, Mathematics Institute, UK, *Computational surface PDEs*, October 31.

28. R. Eymard, Université Paris Est, Département de Mathématiques, Marne-la-Vallée, France, *Low degree nonconforming methods for the biharmonic problem*, January 13.

29. K. Fellner, University of Graz, Institute for Mathematics and Scientific Computing, Austria, *Organic photovoltaic devices, drift-diffusion systems and entropy methods*, September 28.

30. L.A. Fernandez, Universidad de Cantabria, Departamento de Matématicas, Santander, Spain, *Mathematical modeling in cancer and some related optimal control problems*, November 22.

31. K. Filonenko, St. Petersburg State University, V.A. Fock Physics Institute, Russia, *One- and two-frequency spectral purities of optical parametric oscillator*, July 14.

32. Ch.-D. Fuh, Academia Sinica, Institute of Statistical Science, Taipei, Taiwan, *HMM and HAC*, May 25.

33. P. Fulmański, University of Lodz, Faculty of Mathematics and Computer Sciences, Poland, *Level set approach to shape optimization — Numerical analysis*, December 6.

34. F. Gach, University of Cambridge, Department of Mathematics, UK, *Efficiency in indirect inference*, February 9.

35. S. Ganesan, Indian Institute of Science, Supercomputer Education and Research Center, Bangalore, *Finite element simulation of free surface and two-phase flows using moving meshes*, May 30.

36. M. Gerdts, Universität der Bundeswehr München, Institut für Mathematik und Rechneranwendung, Neubiberg, *Optimale Steuerung und parametrische Sensitivitätsanalyse in Fahrerassistenzsystemen*, August 23.

37. G. Gilardi, Università di Pavia, Dipartimento di Matematica, Italy, *Solutions to models of phase segregation — Part 2*, February 6.

38. D. Glyzin, Yaroslavl State University, Department Modeling and Analysis of Information Systems, Russia, *Relaxation oscillations in a chain of coupled delay differential equations*, December 1.

39. K. Götze, Technische Universität Darmstadt, Fachbereich Mathematik, *Strong solutions for the interaction of rigid bodies and viscoelastic fluids*, October 26.

40. M. Grasselli, Politecnico di Milano, Dipartimento di Matematica, Italy, *Recent results on Cahn–Hilliard–Navier–Stokes systems*, May 3.

41. M. Grmela, École Polytechnique de Montréal, Department of Chemical Engineering, Canada, *Geometry of mesoscopic dynamics and thermodynamics*, July 13.

42. S. Gugushvili, Vrije Universiteit Amsterdam, Department of Mathematics, The Netherlands, *$\sqrt{n}$-consistent parameter estimation for systems of ordinary differential equations: Bypassing numerical integration via smoothing*, May 11.

43. S. Gurevich, Westfälische Wilhelms-Universität Münster, Institut für Theoretische Physik, *Destabilization of localized structures induced by delayed feedback*, December 6.

44. Ch.M. Hafner, Université Catholique de Louvain, Ecole de Statistique, Biostatistique et Sciences Actuarielles (LSBA), Belgium, *Volatility of price indices for heterogeneous goods*, November 30.

45. R. Haller-Dintelmann, Technische Universität Darmstadt, Fachbereich Mathematik, *Hardy's inequality for mixed boundary conditions*, December 14.

46. R. Hanke-Rauschenbach, Max-Planck-Institut für Dynamik komplexer technischer Systeme, Fachgruppe Physikalisch-Chemische Prozesstechnik, Magdeburg, *Oscillations and pattern formation in an electrochemical membrane reactor exposed to H_2/CO mixtures*, June 14.

47. Ch. Hellwig, Deutsches Zentrum für Luft- und Raumfahrt, Institut für Technische Thermodynamik, Stuttgart, *Physically based modeling of impedance and discharge behavior of a LiFePo4-based Li-ion battery*, April 19.

48. M. Hirokawa, Okayama University, Graduate School of Natural Sciences and Technology, Department of Mathematics, Japan, *Some mathematical problems on modeling in circuit quantum electrodynamics*, September 7.

49. M. Hofmann, École Nationale de la Statistique et de l'Administration Économique, Malakoff, France, *Statistical inference and financial data modelling across time scales*, January 19.

50. R.H. Hoppe, University of Houston, Department of Mathematics/Universität Augsburg, Institut für Mathematik, USA/Germany, *Optimal diffeomorphic matching of dynamically deformable surfaces and applications in biometrical image processing*, May 18.

51. M. Hoyuelos, Universidad Nacional de Mar del Plata, Facultad de Ciencias Exactas y Naturales, Funes, Argentina, *Entropy of non-equilibrium systems, the case of the Fokker–Planck equation*, March 9.

52. St. Huckemann, Universität Göttingen, Institut für Mathematische Stochastik, *On (semi)-intrinsic statistical analysis of shape*, February 16.

53. G. Huyet, Cork Institute of Technology, Physics Department, Ireland, *Dynamics of quantum dot semiconductor lasers*, July 7.

54. W. Izumida, Tohoku University, Department of Physics, Sendai, Japan, *Curvature effects in rolled-up semiconductor layers and carbon nanotubes*, March 2.

55. A. Jourani, Université de Bourgogne, Département de Mathématiques, Dijon, France, *Controllability and strong controllability of differential inclusions*, September 6.

56. P. Jung, Sogang University, Department of Mathematics, Seoul, Korea, *Random walks at random times*, July 6.

57. ———, *Random time transformations and fractional stable motions*, July 8.

58. G. Kitavtsev, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, *Weak solutions to lubrication equations in the presence of strong slippage*, February 2.

59. P. Knobloch, Charles University, Institute of Numerical Mathematics, Prague, Czech Republic, *Improved stability and error analysis for a class of local projection stabilizations applied to the Oseen problem*, August 30.

60. Th. Kolokolnikov, Dalhousie University, Mathematics and Statistics Department, Halifax, Canada, *Particle interaction models of biological aggregation*, August 9.

61. V. Koltchinski, Georgia Institute of Technology, School of Mathematics, Atlanta, USA, *Von Neumann entropy penalization and low rank matrix estimation*, April 20.

62. R. Kornhuber, Freie Universität Berlin, Institut für Mathematik, *On Ritz–Galerkin methods for stochastic partial differential equations*, April 7.

63. D. Kourounis, Stanford University, Department of Energy Resources Engineering, USA, *Adjoint formulations for gradient-based optimization of compositional flow*, June 21.

64. S. Kpotufe, Max-Planck-Institut für Intelligente Systeme, Abteilung Empirische Inferenz, Tübingen, *The curse of dimension in nonparametric regression*, November 23.

65. M. Kränkel, Universität Freiburg, Abteilung für Angewandte Mathematik, *A local discontinuous Galerkin method for a compressible phase field model*, July 7.

66. P. Krejčí, Academy of Sciences of the Czech Republic, Institute of Mathematics, Prague, *Remarks on uniqueness in quasilinear parabolic systems*, November 2.

67. U. Krewer, Max-Planck-Institut für Dynamik komplexer technischer Systeme, Portable Energiesysteme, Magdeburg, *Influence of reactant transport on electrochemical energy systems*, February 17.

68. M. Kuhn, LightTrans GmbH, Jena, *Unified optical modeling*, May 18.

69. C. Laing, Massey University, Institute of Information and Mathematical Sciences, Auckland, New Zealand, *Fronts and bumps in spatially extended Kuramoto networks*, November 22.

70. O. Lass, T. Seger, Universität Konstanz, Fachbereich Mathematik und Statistik, *Analysis and numerics for an elliptic parabolic system arising in the modeling of batteries and fuel cells*, June 28.

71. A. Latz, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Strömungs- und Materialsimulation, Kaiserslautern, *Thermodynamic consistent modeling and simulations of transport on micro- and nanoscales in Li-ion batteries*, May 16.

72. A. Laurain, Humboldt-Universität zu Berlin, Institut für Mathematik, *Recent advances in shape and topology optimization: Theory and applications*, November 3.

73. J. Lengiewicz, Polish Academy of Sciences, Institute of Fundamental Technological Research, Warsaw, *Continuum formulation and finite element analysis of finite wear*, June 7.

74. M. Löwe, Westfälische Wilhems-Universität Münster, Institut für Mathematische Statistik, *Reconstruction of random scenery — Results an perspectives*, July 13.

75. R. M. Castro, Eindhoven University of Technology, Department of Mathematics, The Netherlands, *Adaptive sensing for sparse signal detection and localization*, November 2.

76. H. Mai, Humboldt-Universität zu Berlin, Institut für Mathematik, *Efficient estimation for a Lévy-driven SDEs and jump filtering*, June 28.

77. M.M. Malamud, Donetsk National University, Department of Mathematics, Ukraine, *On the unitary equivalence of absolutely continuous parts of self-adjoint extensions*, February 16.

78. M. Malioutov, Northeastern University, Department of Mathematics, Boston, USA, *Search for active inputs*, February 22.

79. ———, *Greedy separate testing of sparse inputs*, September 5.

80. St. Mallat, Ecole Polytechnique, Centre de Mathématiques Appliquées, Palaiseau, France, *High dimensional classification with invariant representations*, July 5.

81. P.A. Markowich, Cambridge University, Department of Applied Mathematics and Theoretical Physics, UK, and University of Vienna, Faculty of Mathematics, Austria, Matheon *Special Guest Lecture: On Wigner and Bohmian measures I (survey lecture)*, June 22.

82. ———, Matheon *Special Guest Lecture: On Wigner and Bohmian measures II*, June 24.

83. ———, MATHEON *Special Guest Lecture: On numerical methods for highly oscillatory Schrödinger equations*, June 28.

84. ———, MATHEON *Special Guest Lecture: On PDE models for socio-economic problems (price formation, opinion formation and crowd modeling)*, June 29.

85. S. MATERA, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, *A first-principles based multiscale modeling approach from the electronic to the continuum regime for model catalyst studies*, May 12.

86. G. MATTHIES, Universität Kassel, Institut für Mathematik, *MooNMD — A program package based on mapped finite element methods*, May 5.

87. M. MATVIICHUK, National Taras Sevchenko University of Kiev, Institute of Mathematics, Ukraine, *Some aspects of one-dimensional dynamics. Sharkovsky's theorem*, March 3.

88. TH. MEYER-BRANDIS, Ludwig-Maximilians-Universität München, Mathematisches Institut, *Malliavin differentiability of strong solutions of SDEs with application to the computation of Greeks*, May 18.

89. M. MEYRIES, Karlsruher Institut für Technologie, Institut für Analysis, *Parabolische Probleme mit nichtlinearen Randbedingungen*, May 18.

90. ———, *Optimal Sobolev embeddings and interpolation with boundary conditions for a class of weighted function spaces*, December 7.

91. G.L. MILLER, Carnegie Mellon University, Computer Science Department, Pittsburgh, USA, *Algorithm design using spectral graph theory*, June 17.

92. S. MOHAMMED, Southern Illinois University, Department of Mathematics, USA, *Linear stochastic partial differential equations*, July 26.

93. J. NAUMANN, Humboldt-Universität zu Berlin, Institut für Mathematik, *On the existence of weak solutions to Prandtl's (1945) turbulence model*, February 16.

94. ———, *On Prandtl's turbulence model: Existence of weak solutions to the equations of turbulent pipe-flow*, November 16.

95. J. NOVO, Universidad Autonoma de Madrid, Instituto de Ciencias Matemáticas, Spain, *Mixed finite-element approximations to the Navier–Stokes equations: Two-grid schemes and a posteriori error estimations*, November 3.

96. J. OUTRATA, Academy of Sciences of the Czech Republic, Institute of Information Theory and Automation, Prague, *Second-order variational analysis and its applications*, September 6.

97. G. PAASCH, Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Abteilung "Elektronische und optische Eigenschaften", *Gaussian transport states in organic devices*, December 1.

98. V. PANOV, Universität Duisburg Essen, Fachbereich Mathematik, *Abelian theorem for stochastic volatility models and semiparametric estimation of the signal space*, November 22.

99. L. PAOLI, Université de Saint-Etienne, Laboratoire de Mathématiques, France, *Asymptotic behaviour of a micropolar fluid flow in a thin domain with a rough boundary*, February 9.

100. V. PATILEA, Ecole Nationale de la Statistique et de l'Analyse de l'Information, Campus de Ker-Lann, Bruz, France, *Adaptive estimation of VaR with time-varying variance : Application to testing linear causality in mean and VaR order*, June 1.

101. W. PROCHAZKA, Kompetenzzentrum Das Virtuelle Fahrzeug Forschungsgesellschaft mbH, Graz, Austria, *Elektrochemische Lithiumionen Zellsimulation am Virtuellen Fahrzeug*, May 3.

102. D.A. PUZYREV, St. Petersburg State University, Department of Computational Physics, Russia, *Advanced numerical and computational methods in modeling of quantum few-body phenomena*, July 5.

103. A. Ramm, Kansas State University, Mathematics Department, Manhattan, USA, *Wave scattering by many small bodies (particles) and creating materials with a desired refraction coefficient*, May 24.

104. M.G. Rasmussen, Aarhus University, Department of Mathematical Sciences, Denmark, *Scattering theory for the translation-invariant Nelson and polaron models: Asymptotic completeness below the two-boson threshold*, March 23.

105. P. Reynaud-Bouret, Université de Nice Sophia-Antipolis, Laboratoire de Mathématiques J.A. Dieudonné, France, *Hawkes process as models for some genomic data*, July 13.

106. M. Roberts, Université Pierre et Marie Curie (Paris VI), Laboratoire de Probabilités, France, *A simple path to asymptotics for the frontier of a branching Brownian motion*, June 20.

107. E. Rocca, Università degli Studi di Milano, Dipartimento di Matematica "F. Enriques", Italy, *On a quasilinear multi-phase system with nonconstant specific heat and heat conductivity*, February 8.

108. M. Rosenbaum, Centre de Recherche en Économie et Statistique (CREST), Paris, France, *Asymptotic results for time-changed Lévy processes sampled at hitting times*, February 2.

109. R. Rossi, Università di Brescia, Dipartimento di Matematica, Italy, *WED functionals for gradient flows in metric spaces: The convex case*, February 21.

110. ———, *A model for adhesive contact with friction*, May 25.

111. T. Roubíček, Charles University, Mathematical Institute, Prague, Czech Republic, *Perfect plasticity at small strains and its thermodynamics*, February 2.

112. K. Sandfort, Karlsruher Institut für Technologie, Fakultät für Mathematik, *Scattering from periodic media and first ideas for scattering from bounded, uniformly patterned media*, January 11.

113. C. Schillings, Universität Trier, Fachbereich IV — Mathematik, *Optimal aerodynamic design under uncertainty*, November 28.

114. K. Schmidt, Technische Universität Berlin, Institut für Mathematik, *High order transmission conditions for conductive thin sheets*, June 1.

115. A. Schröder, Humboldt-Universität zu Berlin, Institut für Mathematik, *Numerical analysis for a vanishing viscosity fracture model*, January 26.

116. A. Segatti, Università degli Studi di Pavia, Dipartimento di Matematica, Italy, *Some observation on an ultra-fast diffusion equation with application to phase transition problems*, May 17.

117. J. Shewchuk, University of California at Berkeley, Computer Science Division, USA, *Theoretically guaranteed Delaunay mesh generation — In practice*, September 6.

118. ———, *Dynamic local remeshing for elastoplastic simulation*, September 8.

119. St. Siegmund, Technische Universität Dresden, Institut für Analysis, *Dynamics in transport, control and systems biology*, February 4.

120. P.X.K. Song, University of Michigan, School of Public Health, USA, *Composite likelihood Bayesian information criterion for model selection in high dimensional correlated data*, May 4.

121. R. Song, University of California at Berkeley, Department of Statistics, USA, *Large vector auto regressions*, April 27.

122. K. Staliunas, Universitat Politecnica de Catalunya, Departament de Fisica i Enginyeria Nuclear, Barcelona, Spain, *Faraday patterns in nonlinear fiber resonators*, December 8.

123. U. Stefanelli, Istituto di Matematica Applicata e Tecnologie Informatiche, Consiglio Nazionale delle Ricerche, Pavia, Italy, *An invitation to shape flows*, May 4.

124. P. Strasser, Technische Universität Berlin, Technische Chemie — Elektro-chemische Katalyse, Energie und Materialwissenschaften Gruppe, *Degradation of Pt and Pt alloy nanoparticle catalysts monitored in situ by X-rays*, June 27.

125. G. Thäter, Karlsruher Insitut für Technologie, Institut für Angewandte und Numerische Mathematik, *Auf Eulers Spuren im Dienste des Hochleistungsrechnens*, November 24.

126. E.S. Titi, University of California, Department of Mathematics, Irvine, USA, *On the loss of regularity for the three-dimensional Euler equations*, January 26.

127. A. Torcini, Institute for Complex Systems, Florence, Italy, *Collective chaos in pulse-coupled neural networks*, February 17.

128. H. Tran, University of Pittsburgh, Mathematics, USA, *Uncoupling the incompressible fluid flows in multi-physics and multi-domain applications*, December 8.

129. M. Tretyakov, University of Leicester, Department of Mathematics, UK, *Numerical integration of Heath–Jarrow–Morton model of interest rates*, September 20.

130. D. Turaev, Imperial College London, Department of Mathematics, UK, *Diffeomorphisms not conjugate to those of higher smoothness*, July 26.

131. M. Vidovic, Technische Universität Berlin, Institut für Mathematik, *Motiverkennung mit POIMs*, July 12.

132. St. Volkwein, Universität Konstanz, *Model reduction for nonlinear problems: Analytical and numerical aspects*, June 27.

133. M. Wagemaker, Technical University Delft, Reactor Institute, The Netherlands, *Dynamic solubility limits in the Li-ion battery electrode material LiFePO4*, March 28.

134. Th. Wagenknecht, University of Leeds, Department of Applied Mathematics, UK, *Homoclinic snaking: Different ways to kill the snakes*, December 13.

135. F. Weidemann, Humboldt-Universität zu Berlin, Institut für Mathematik, *A generalisation of the Hobson–Rogers model*, January 11.

136. G. Witterstein, Technische Universität München, Zentrum Mathematik — M6, *Two-phase compressible fluids*, July 11.

137. M. Yamamoto, University of Tokyo, Department of Mathematical Sciences, Japan, *Reconstruction of a moving boundary from Cauchy data in heat equation*, March 14.

138. ———, *Mathematical analysis for inverse problems in the time cone method*, September 27.

139. M. Yvinec, Institut National de Recherche en Informatique et en Automatique (INRIA), Geometrica project team, France, *Anisotropic Delaunay meshes*, May 26.

140. S. Zelik, University of Surrey, Faculty of Engineering and Physical Sciences, Department of Mathematics, Guildford, UK, *Infinite-dimensionality in the "finite-dimensional" dissipative dynamics*, December 13.

141. E. Zhang, Oregon State University/Berlin Mathematical School, *Topological analysis and visualization of 2D asymmetric tensor fields*, December 6.

142. Y. Zhang, Michelin Americas Research and Development Company, Mountville, SC, USA, *Mathematical modeling and numerical simulations on some tire-related problems*, November 16.

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/).

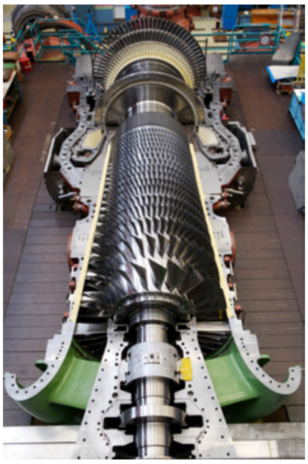
BOP (contact: J. Borchardt, phone: +49 30/20372-485, e-mail: juergen.borchardt@wias-berlin.de)

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 (dMRI) and high angular resolution diffusion-weighted MR imaging (HARDI) data. It can be used to read dMRI data, to estimate the diffusion tensor, for adaptive smoothing of dMRI data, the estimation of orientation density functions, the estimation of tensor mixture models, fiber tracking, 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. The package is 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

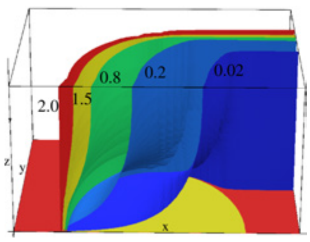
- the availability of more than 100 finite elements in one, two, and three space dimensions (conforming, non-conforming, discontinuous, higher-order, isoparametric, with bubbles)
- the use of implicit time-stepping schemes (θ-schemes, DIRK schemes, Rosenbrock–Wanner schemes)
- the application of a multiple-discretization multi-level (MDML) preconditioner in Krylov subspace methods

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.

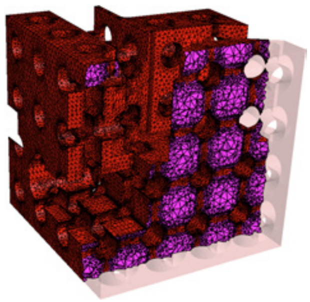


Concentration isosurfaces in a thin-layer flow cell

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 cut view of a constrained Delaunay tetrahedral mesh of a complex 3D solid generated by TetGen

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-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.